Argonne NATIONAL LABORATORY

Applied Mathematics

Argonne Leads the Way in Computational Materials

Computer Science Research at Argonne

Leveraging ALCF Resources

Accelerating Breakthrough Science at the ALCF

Big Data at Argonne

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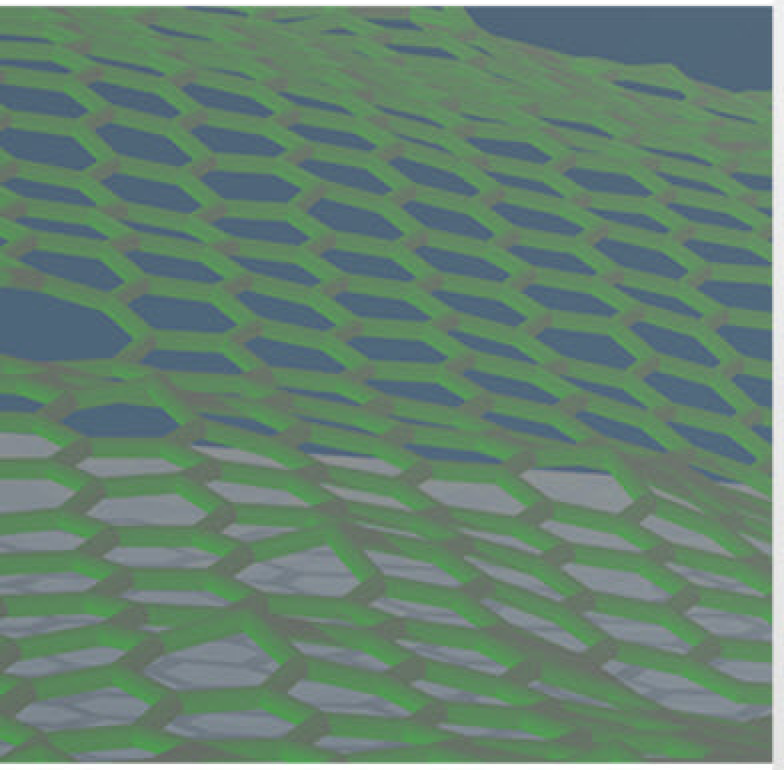

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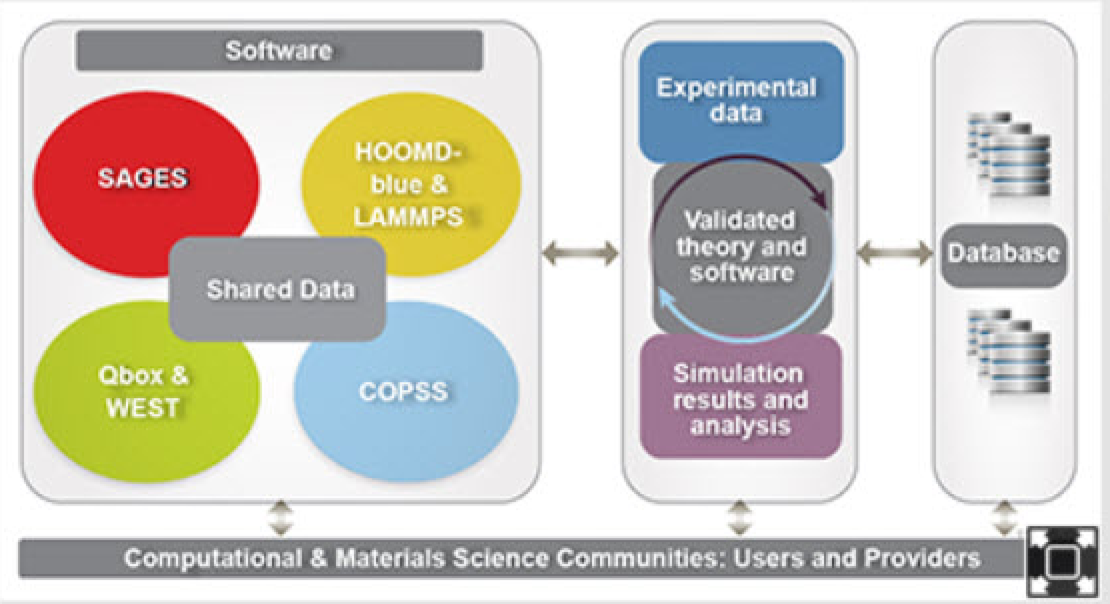
Argonne Leads the Way in Computational Materials

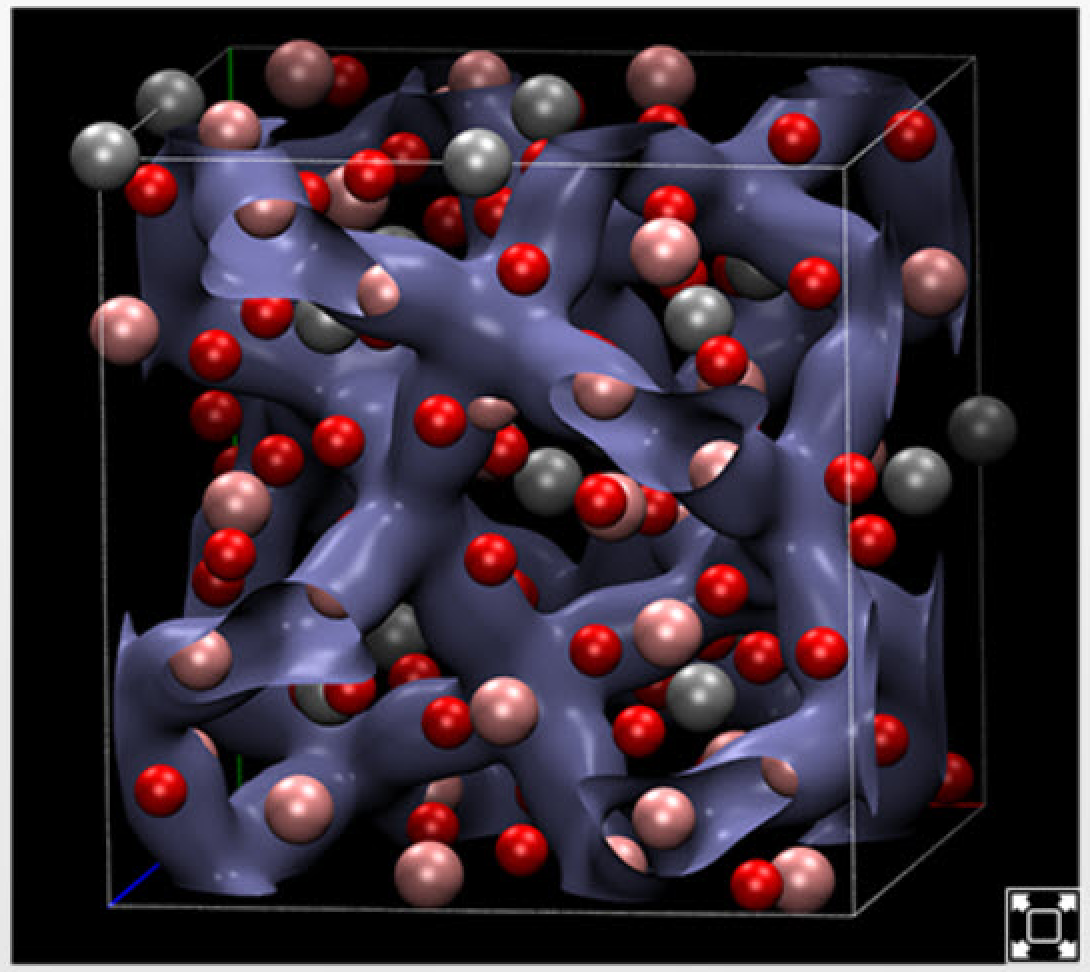
Argonne is leading engineering research and education in new directions, solving major technological problems of global significance, and continually inspiring creative applications of materials science.

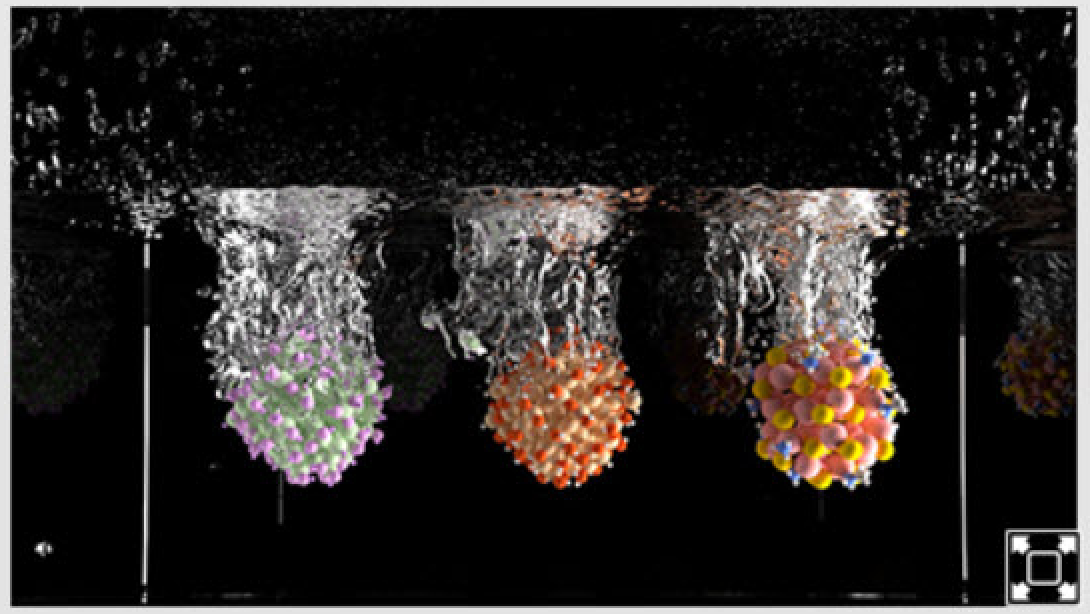
Key centers and initiatives have been established at Argonne to develop breakthrough materials from battery electrodes to self-assembled nanostructures.
Joint Center for Energy Research |Center for Electrochemical Energy Systems | Center for Nanoscale Materials | Institute for Molecular Engineering | Midwest Integrated Center for Computational Materials

DOE creates new Center for Computational Materials at Argonne
The Midwest Integrated Center for Computational Materials (MICCoM) led by DOE's Argonne National Laboratory, develops and disseminates open source software, data, simulation codes and validation procedures, enabling the community to simulate and predict properties of functional materials for energy conversion processes.

MICCoM's emphasis is on interfaces, the transport across them, and the manipulation of matter under conditions far from equilibrium.







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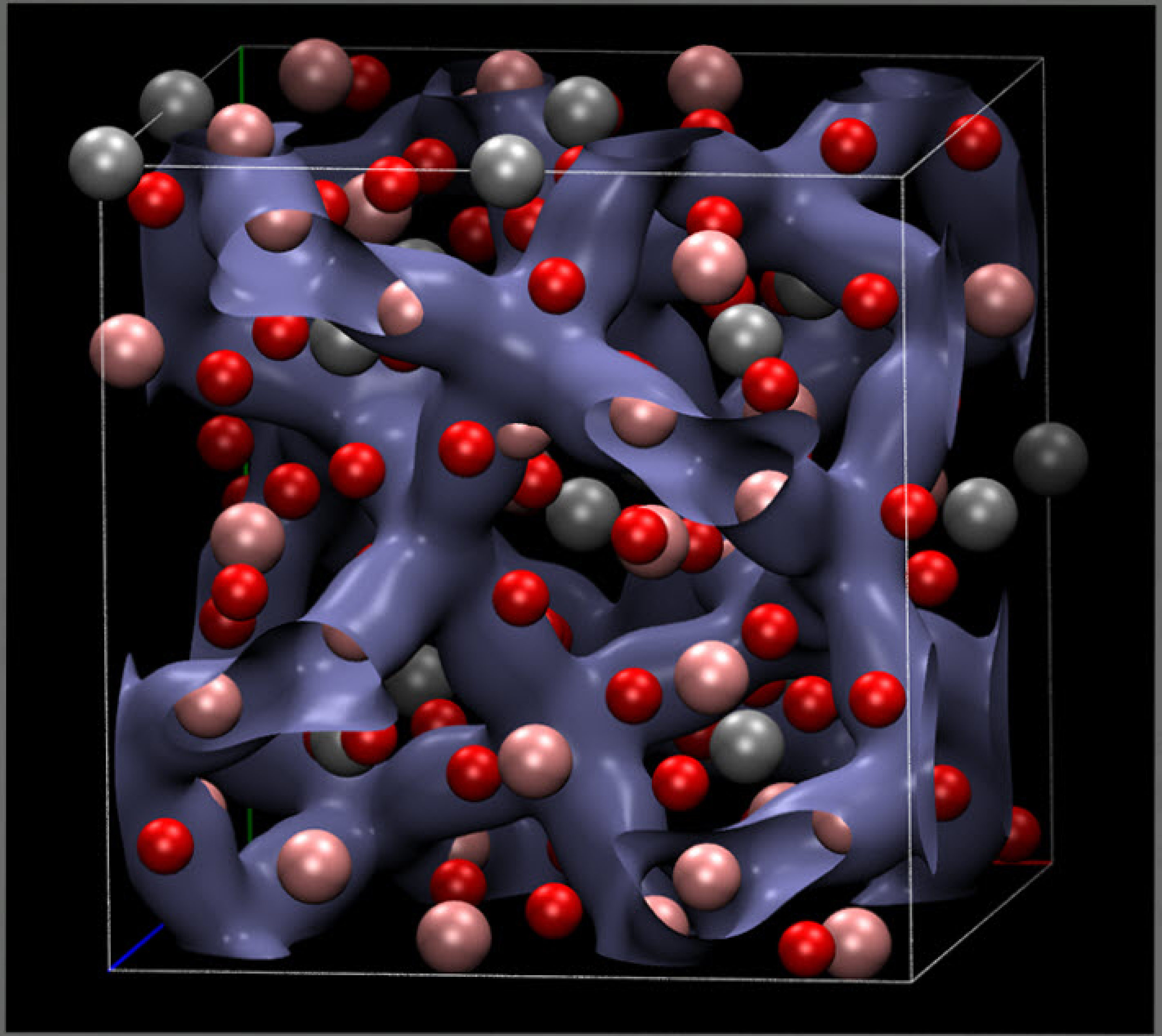
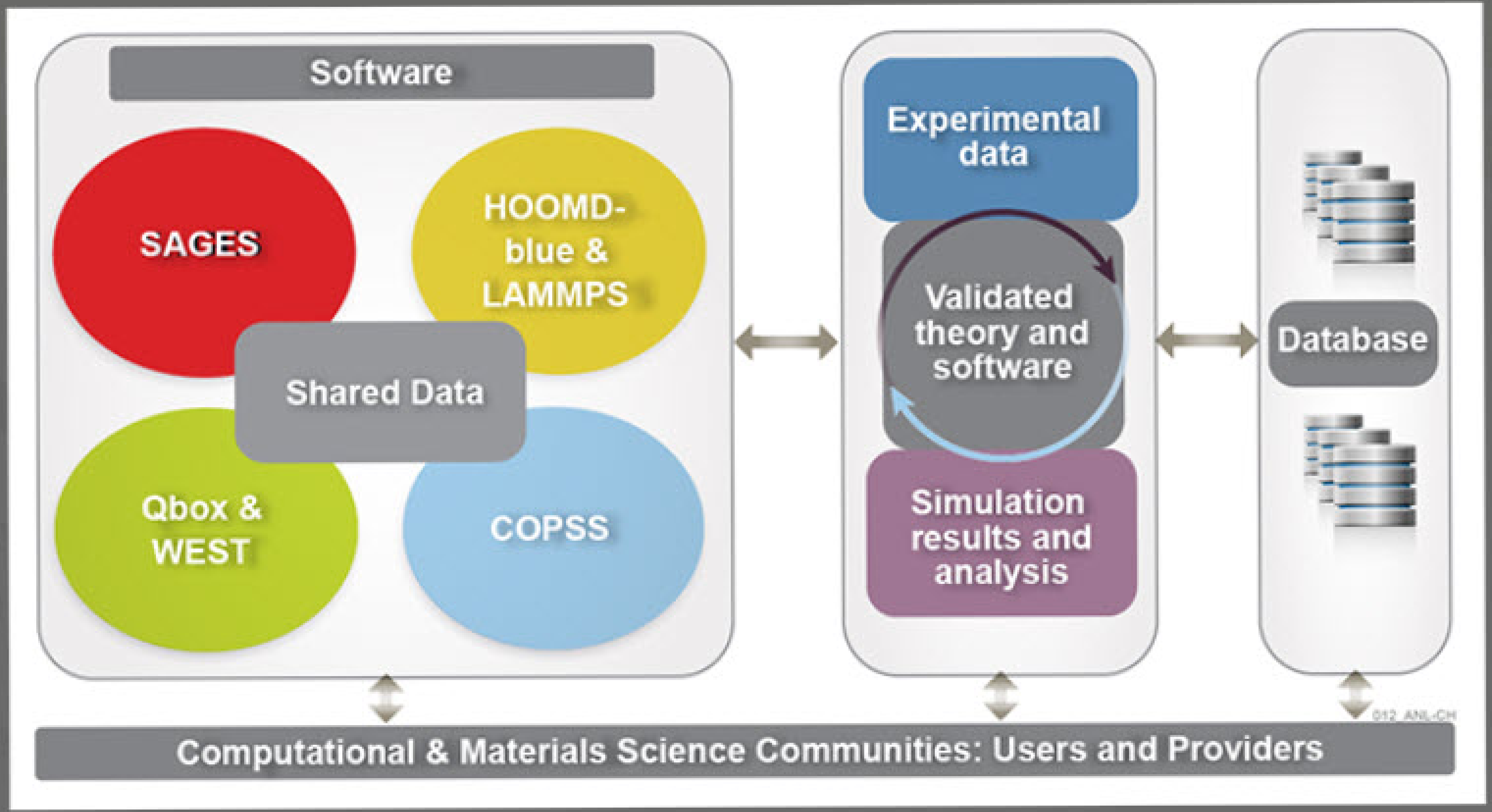


Large-scale simulations are being used to address the key challenges of understanding the physical and chemical mechanisms that will lead to the needed materials breakthroughs for Li-air batteries. PI: Larry Curtiss, Argonne National Laboratory



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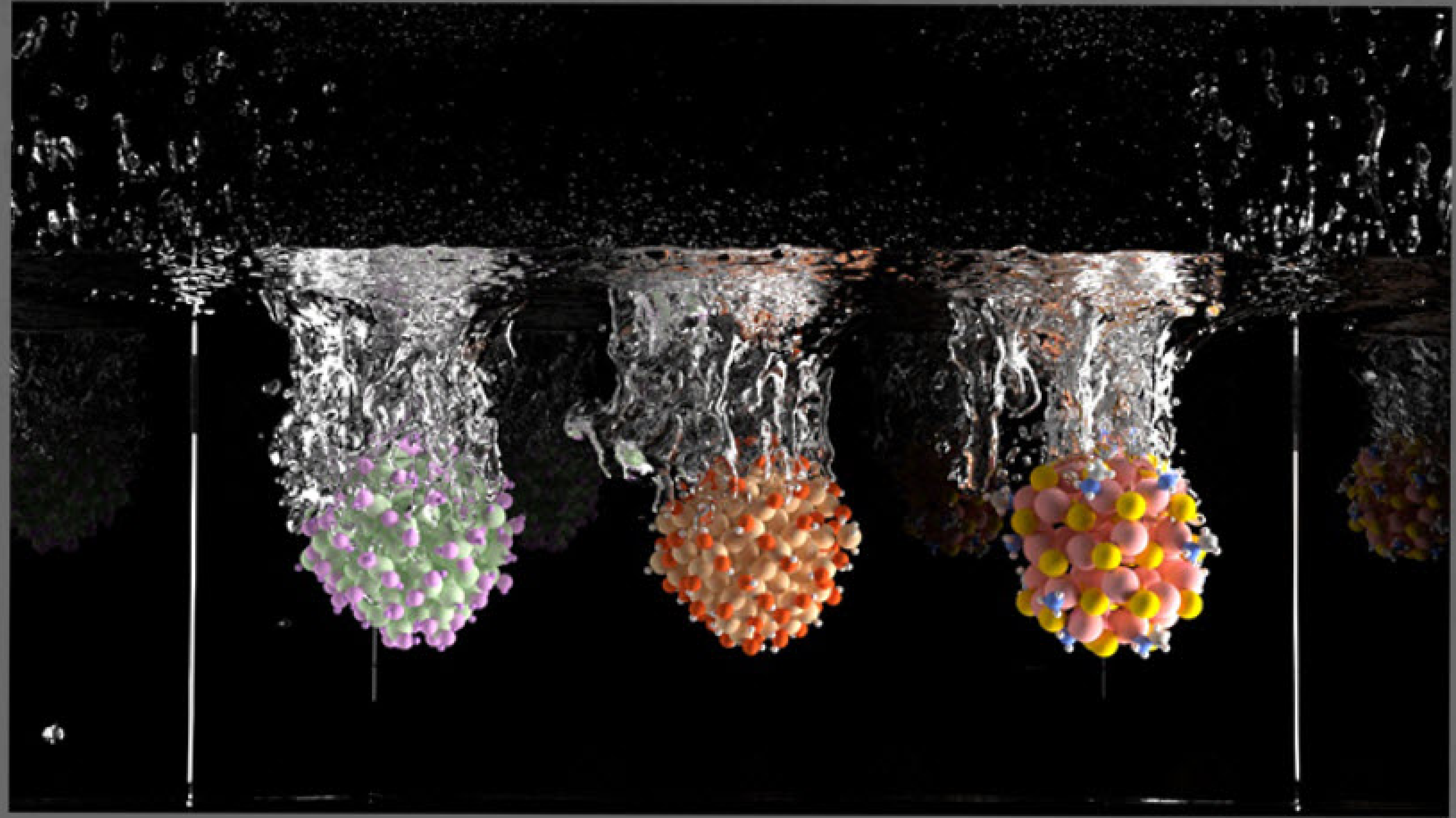
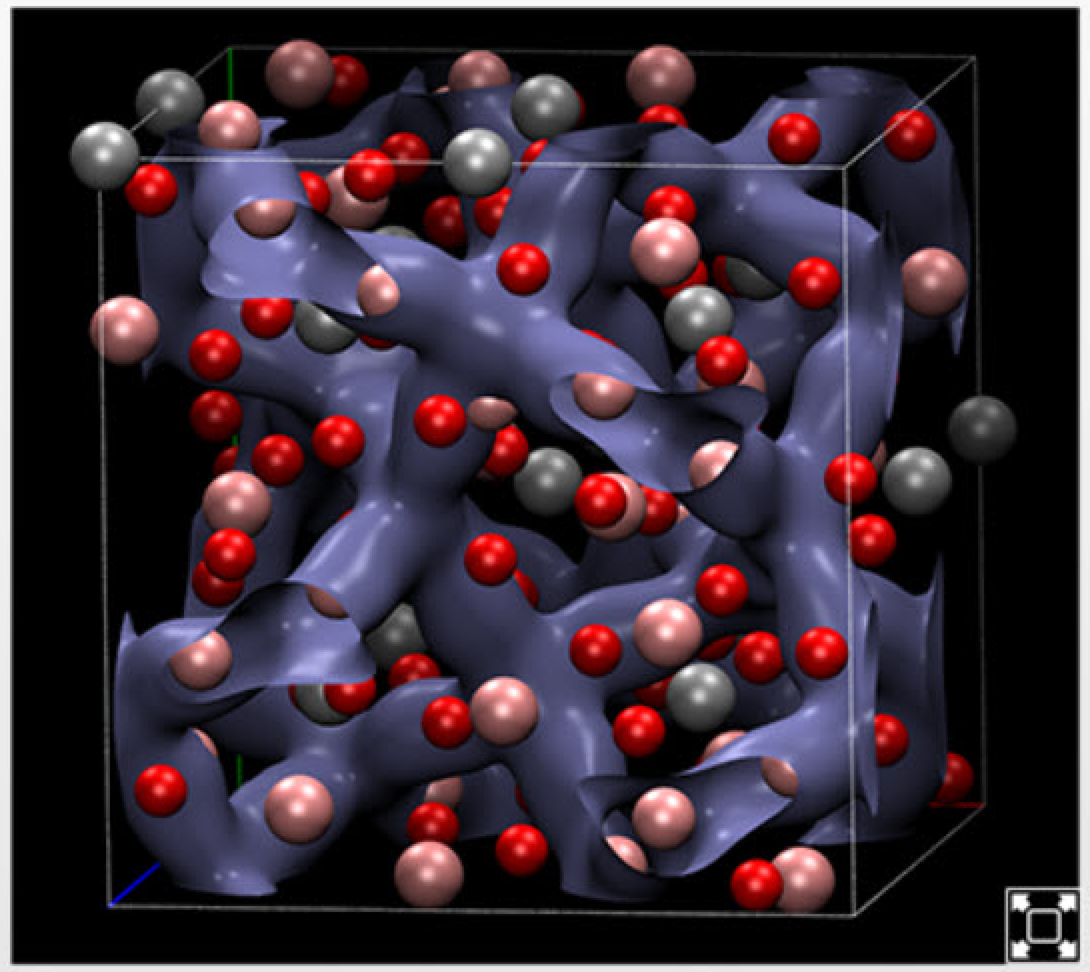
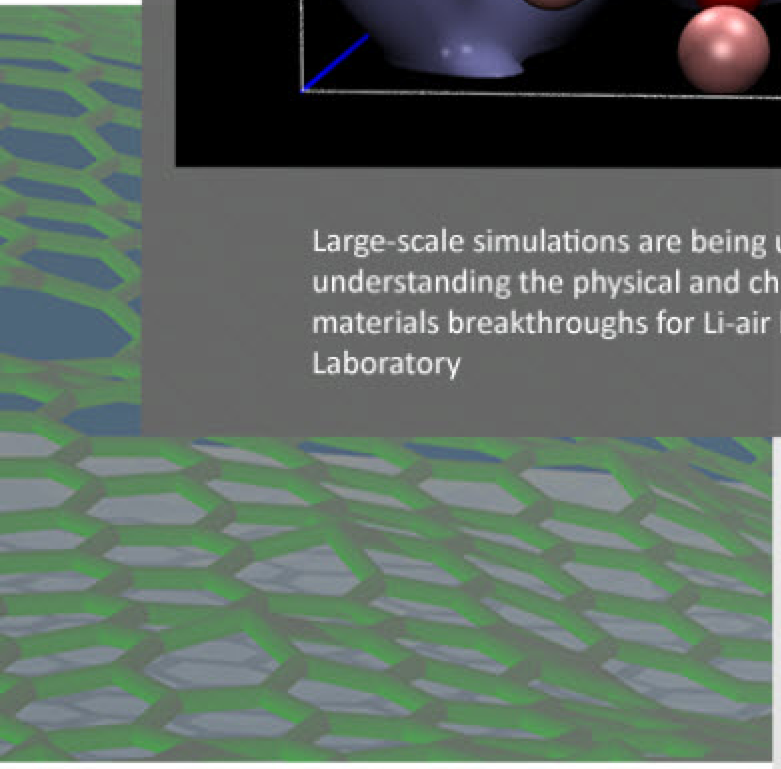


Researchers are combining ab initio molecular dynamics and post-density functional theory methods to optimize properties of nanostructured materials for use in solar and thermal energy conversion devices at an unprecedented level of accuracy. PI: Guilia Galli, University of Chicago.





FUNDING AGENCY: DOE Office of Science

CONTACT: Ray Bair, rbair@anl.gov

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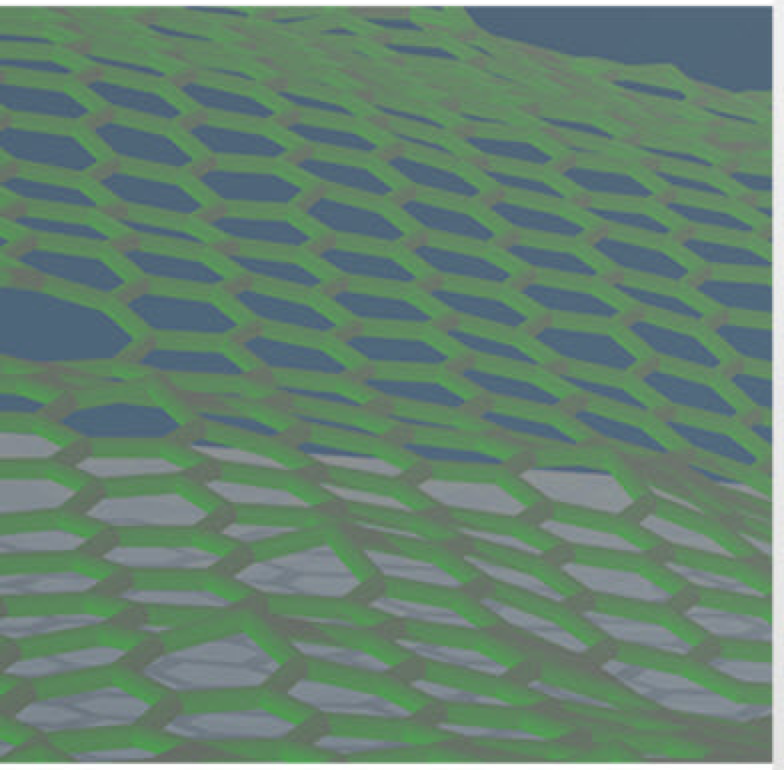

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Computer Science Research at Argonne

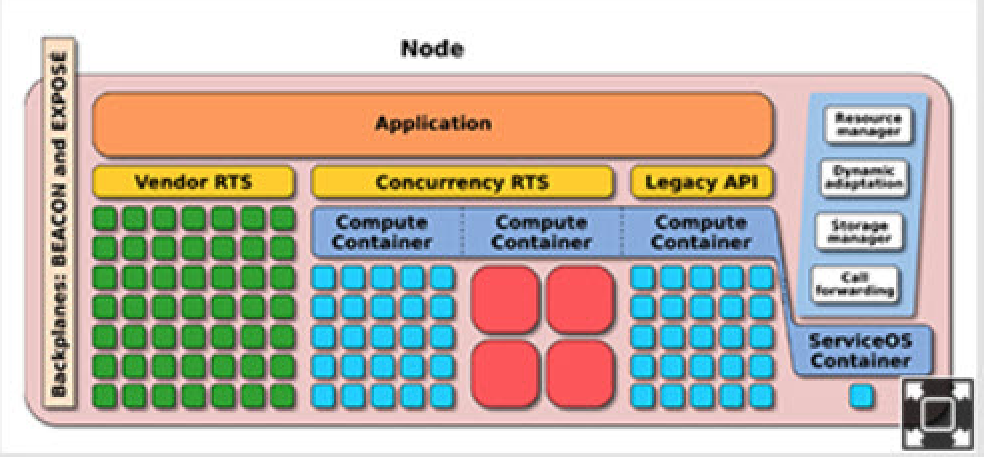
Computer science research at Argonne comprises all aspects of system software for extreme-scale systems (operating systems, runtime, storage, programming models, algorithms, libraries, resilience, and fault tolerance), large-scale data analysis, visualization, scientific workflows, as well as the intersection of cloud and high-performance computing.
http://www.mcs.anl.gov/research

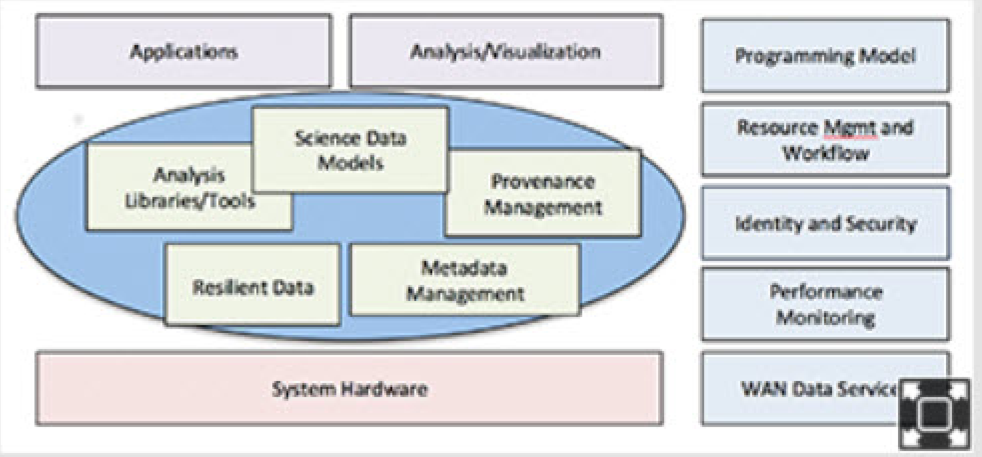
Argo: Operating System for Exascale Computing
Argonne researchers, in collaboration with other partners, are developing an operating system and runtime, called Argo, for future exascale computing systems.
http://www.argo-osr.org

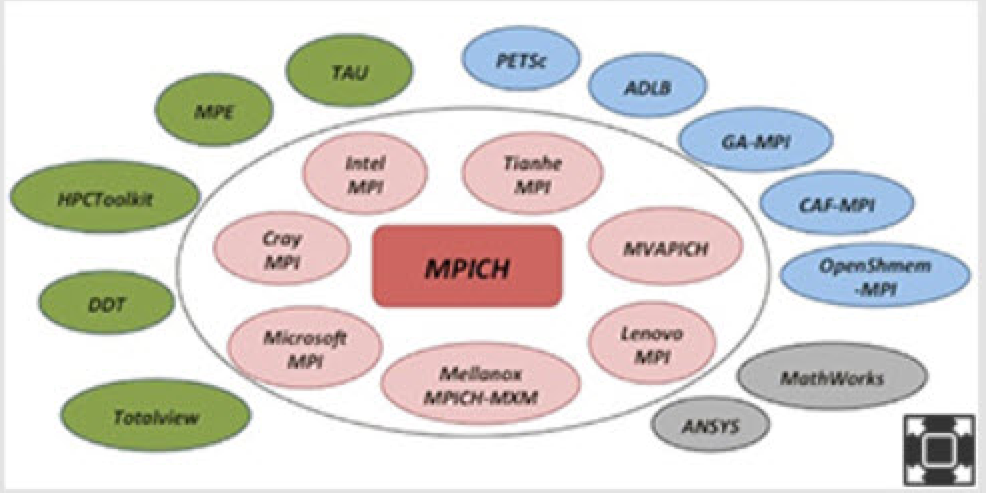
Data-Intensive Science
The task of managing and gaining insight from the petabytes of data produced by large-scale simulations and experiments is one of the most pressing challenges of our time. At Argonne, we are tackling this challenge by developing new techniques and tools for storing, transferring, accessing, visualizing, and analyzing extremely large datasets.
http://www.mcs.anl.gov/group/data-intensive-science

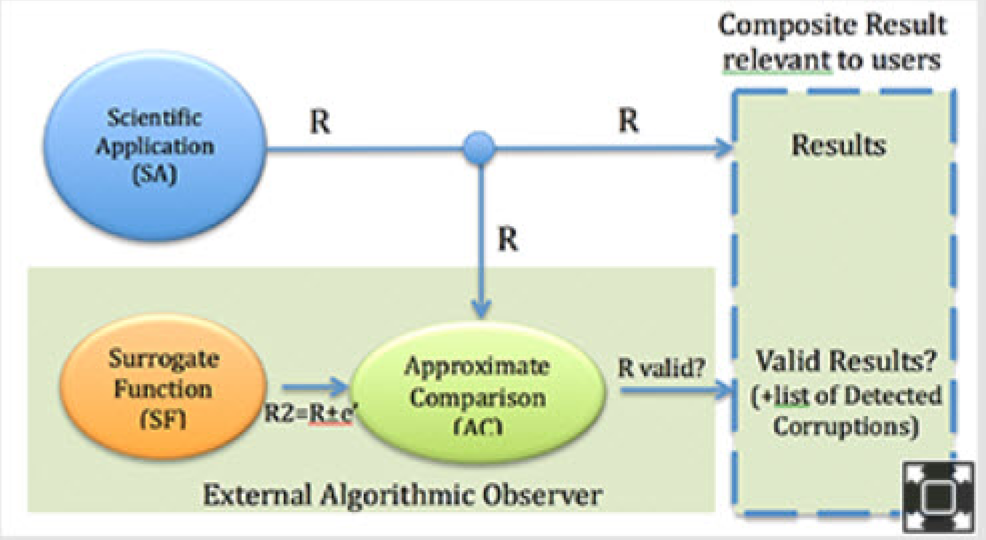
MPICH: The MPI Implementation for Exascale
Researchers at Argonne are the main developers of the widely used MPI implementation MPICH, a winner of the R&D 100 award. MPICH and its derivatives are used in production on 9 of the top 10 supercomputers in the world and hence form the basis of many large-scale scientific simulations.
http://www.mpich.org

Resilience and Fault Tolerance in Scientific Applications
Argonne researchers are developing techniques for detecting Silent Data Corruption (SDCs) in computations. In the figure, the External Algorithmic Observer performs and reports SDC detection by running a low complexity surrogate function and by approximately comparing its result to the one of the scientific application.
https://collab.cels.anl.gov/display/ESR









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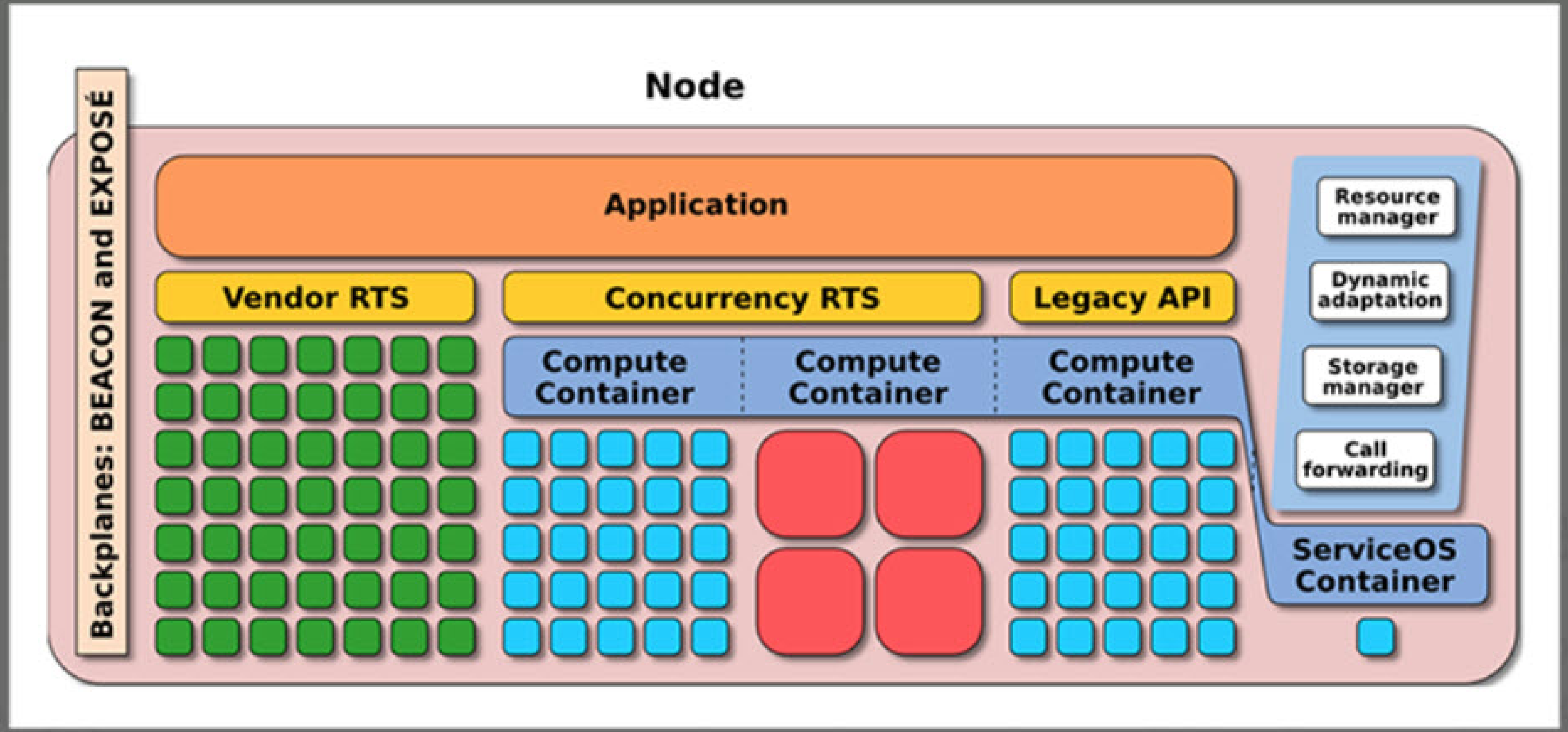

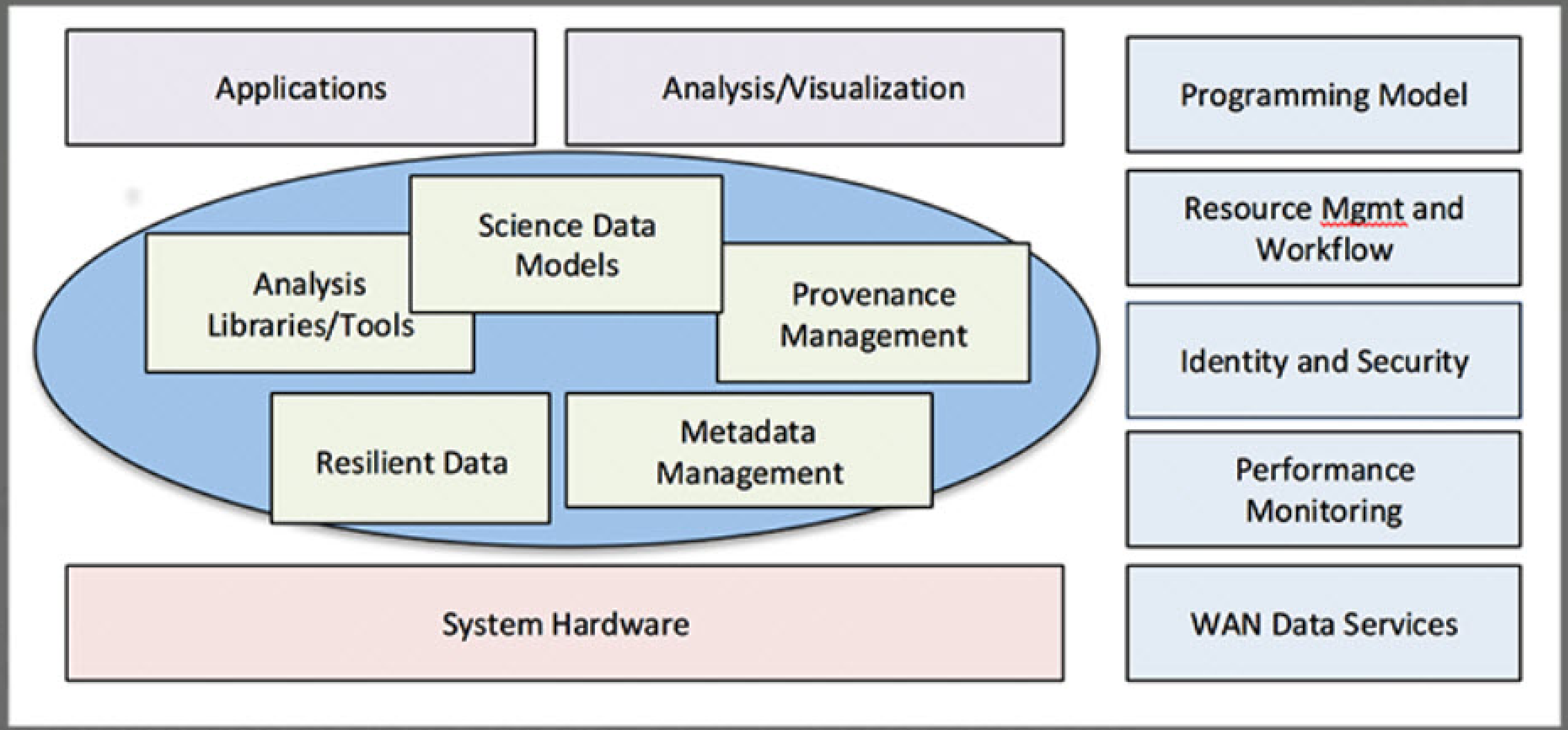

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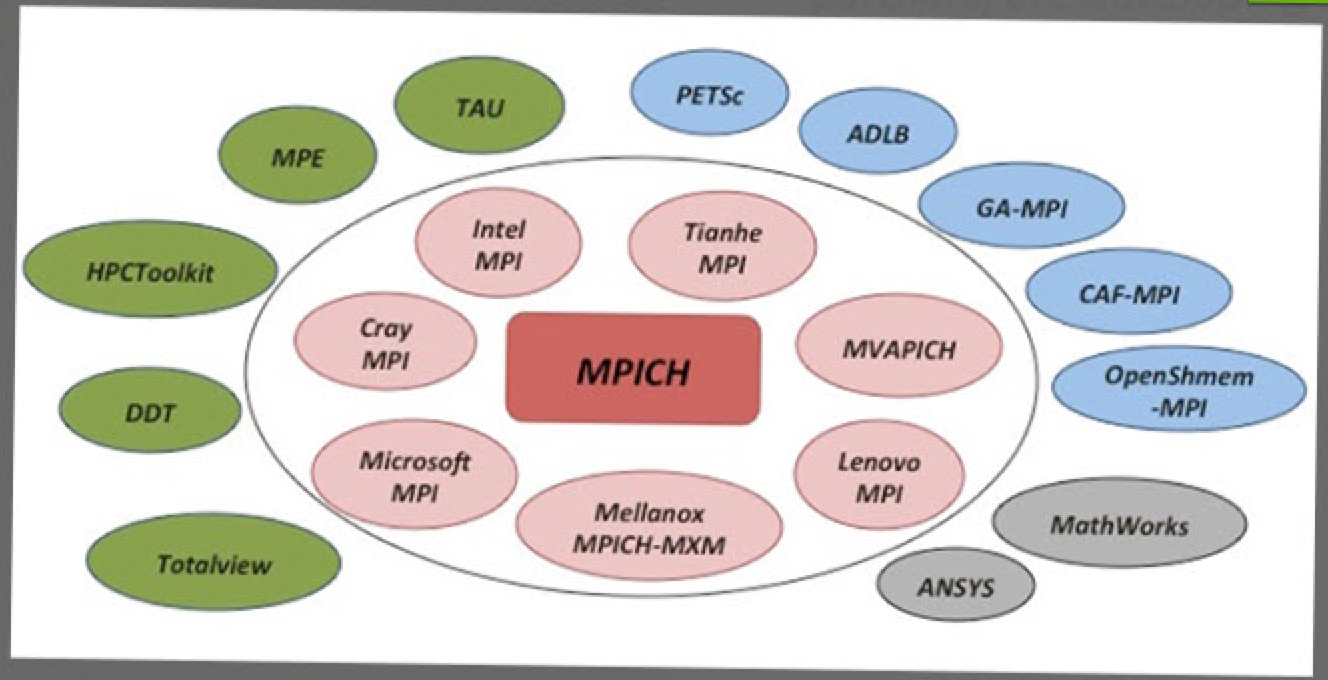

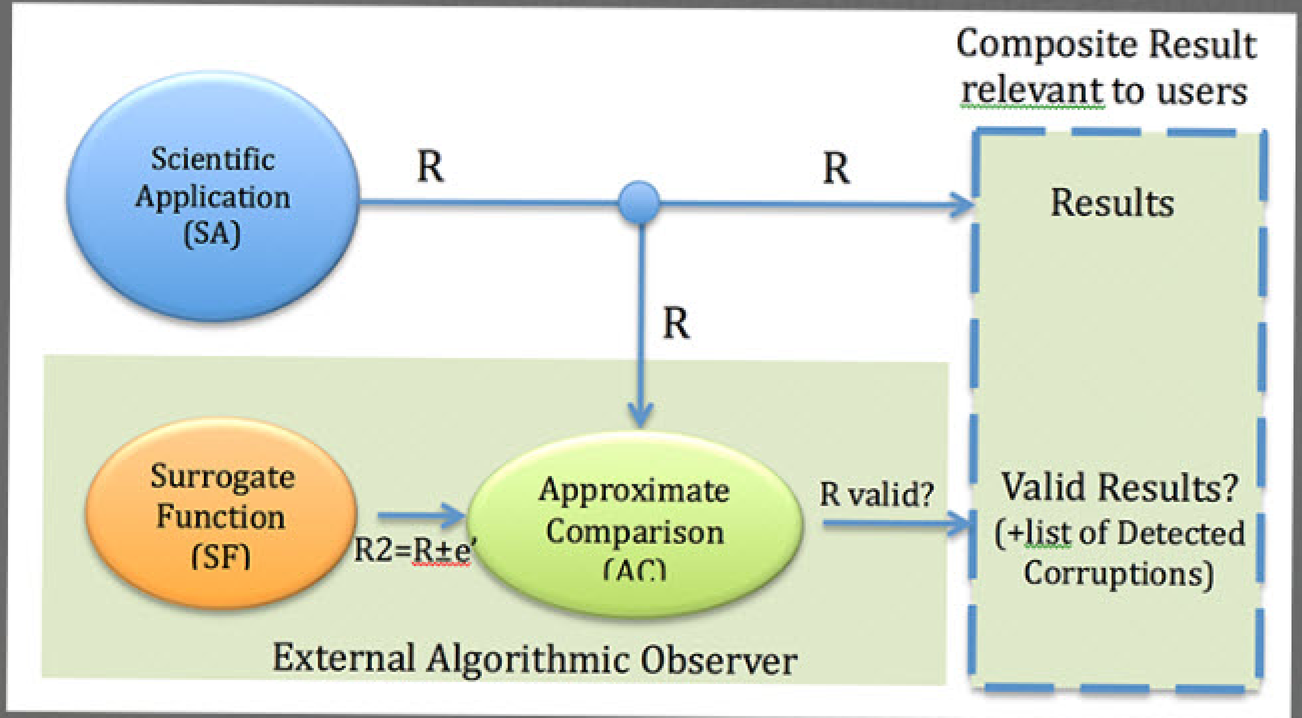

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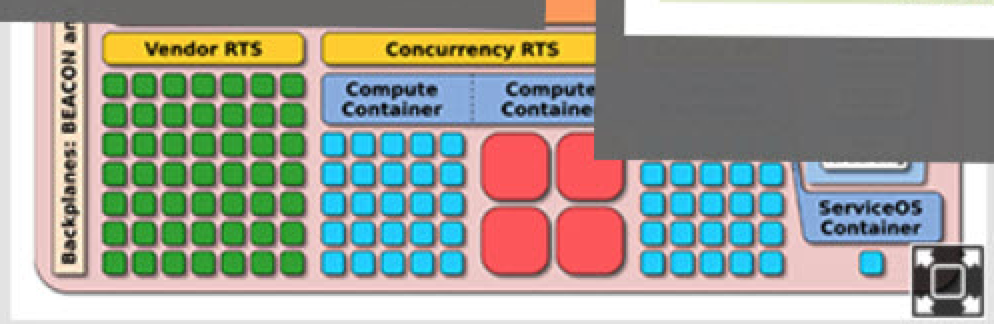
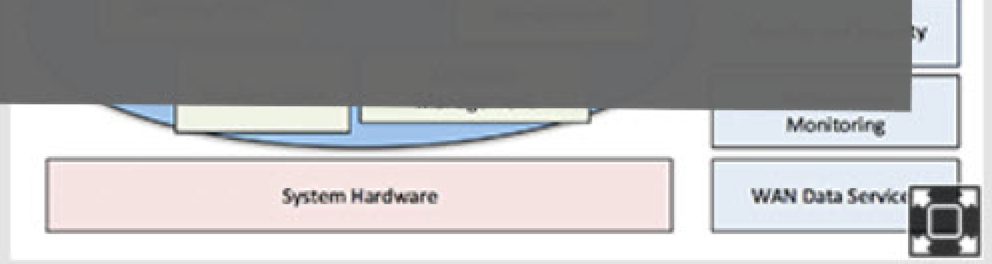
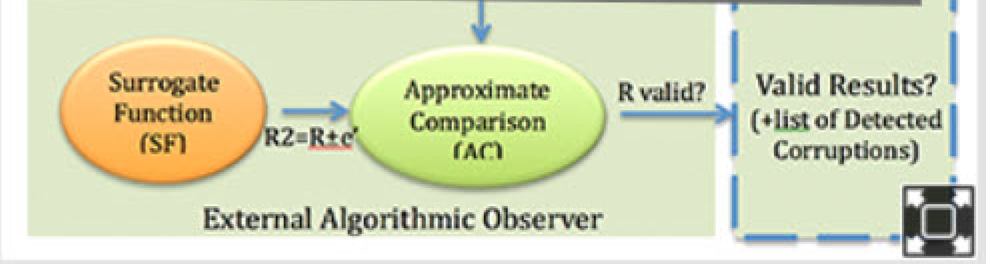
CONTACT: Rajeev Thakur, Pete Beckman, Rob Ross, Pavan Balaji, Franck Cappello, Argonne National Laboratory, [thakur, beckman, rross, balaji, cappello] @mcs.anl.gov







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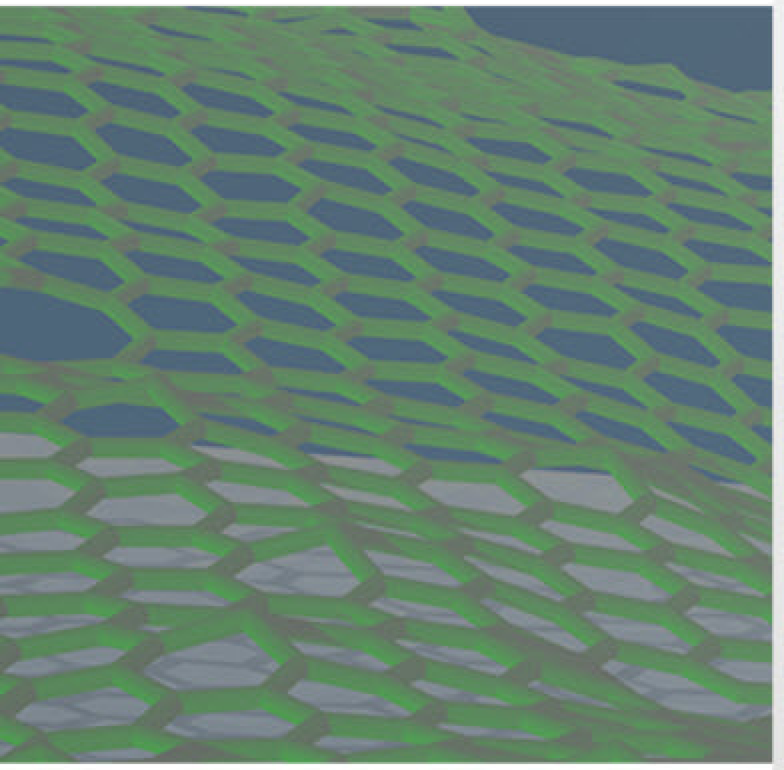

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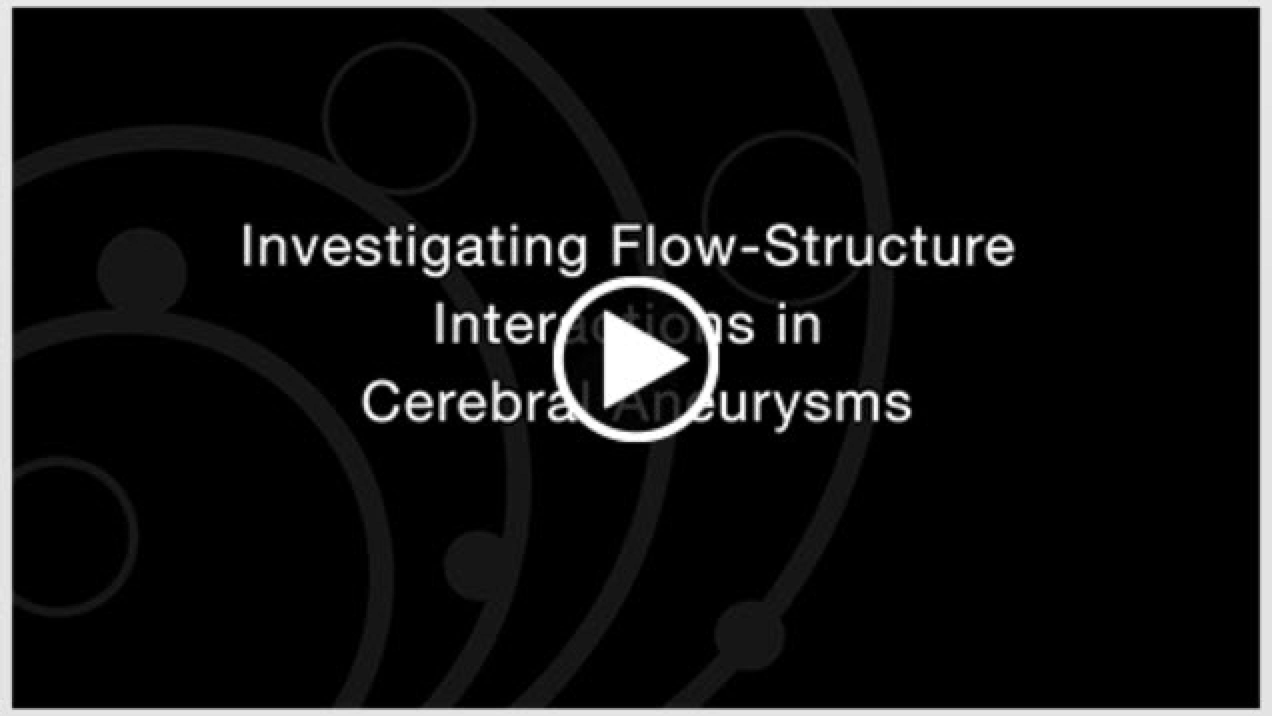
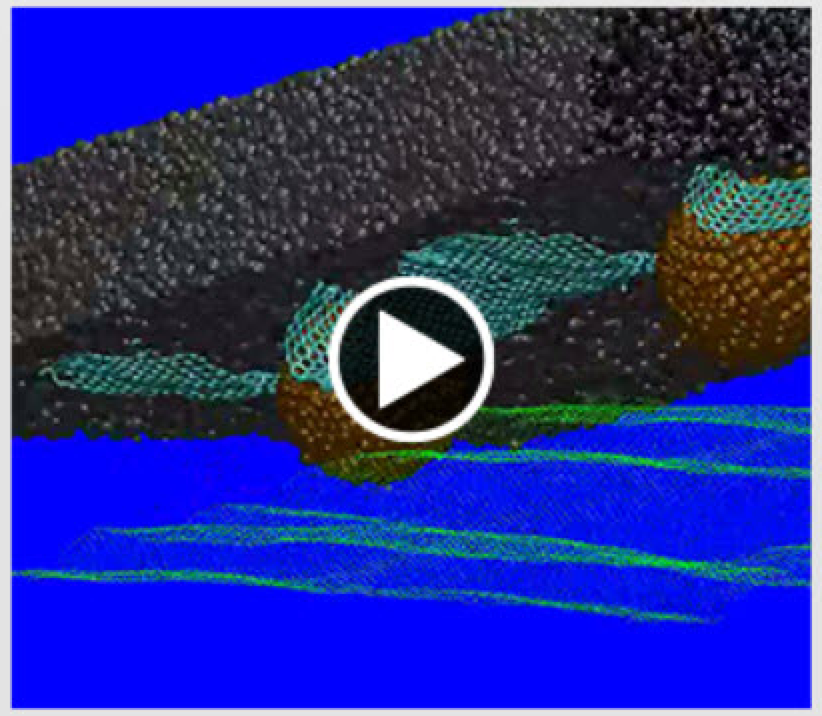
Accelerating Breakthrough Science at the ALCF

The Argonne Leadership Computing Facility (ALCF) provides supercomputing capabilities to the scientific and engineering community to advance fundamental discovery and understanding in a broad range of disciplines. Available to researchers from universities, industry, and government agencies, the ALCF is a national scientific user facility that helps accelerate the pace of discovery and innovation by providing supercomputing resources that are 10 to 100 times more powerful than systems typically available for open scientific research.

Reactive MD Simulations of Electrochemical Oxide Interfaces at Mesoscale
Superlubricity—a state in which friction essentially disappears—is a highly desirable property. Considering that nearly one-third of every fuel tank is spent overcoming friction in automobiles, a material that can achieve superlubricity would greatly benefit industry and consumers alike. Argonne scientists used Mira to identify and improve a new mechanism for eliminating friction, which fed into the development of a hybrid material that exhibited superlubricity at the macroscale for the first time. PI: Subramanian Sankaranarayanan, Argonne National Laboratory.



Multiscale Simulations of Human Pathologies
Thoracic aortic aneurysm and dissection occurs when an aneurysm in the aorta expands and causes a tear in the artery wall. To help better understand and treat this life-threatening condition, are using Mira to perform pioneering multiscale simulations of these aneurysms. By significantly increasing our understanding of thoracic aortic aneurysm and dissection, this research has the promise to lead to an improved prognostic capability and interventional planning. In addition, insight gained in this study will have important implications for a host of other vascular conditions, providing information that could contribute to improved treatments for a broad class of clinical problems. PI: George Karniadakis, Brown University.



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Cerebral aneurysms (CAs) occur in up to 5% of the general population, leading to strokes for over 40,000 Americans each year. Rupture of a CA can be a devastating event that leaves over 60% of afflicted patients dead or disabled. Currently, there exists no formal framework for the diagnosis of CAs. Moreover, assessing the risk of a potential rupture is far from being fully understood. However, it is believed that factors such as location, geometry, blood flow patterns and resulting mechanical stresses within the aneurysm play a prominent role.

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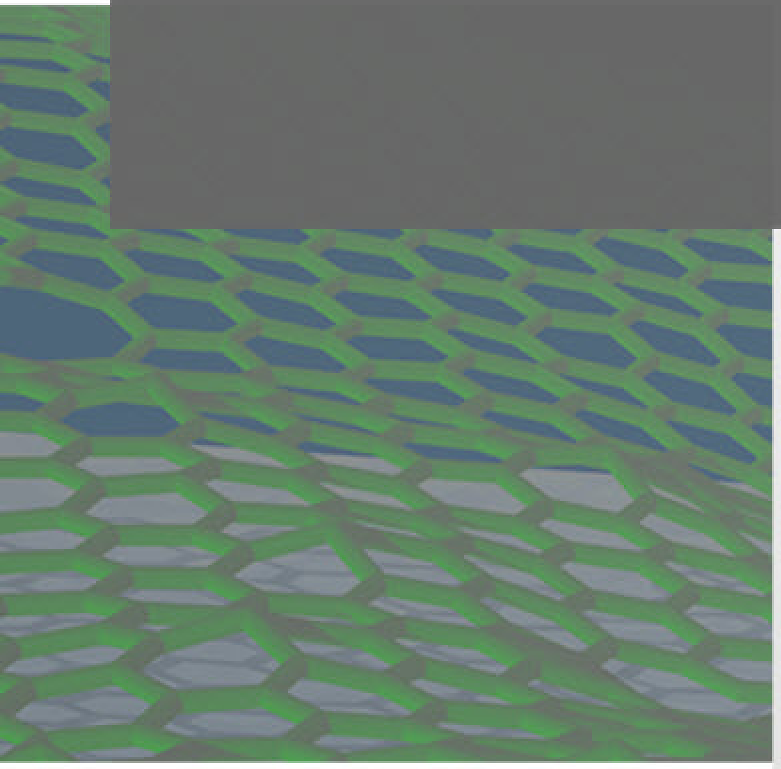

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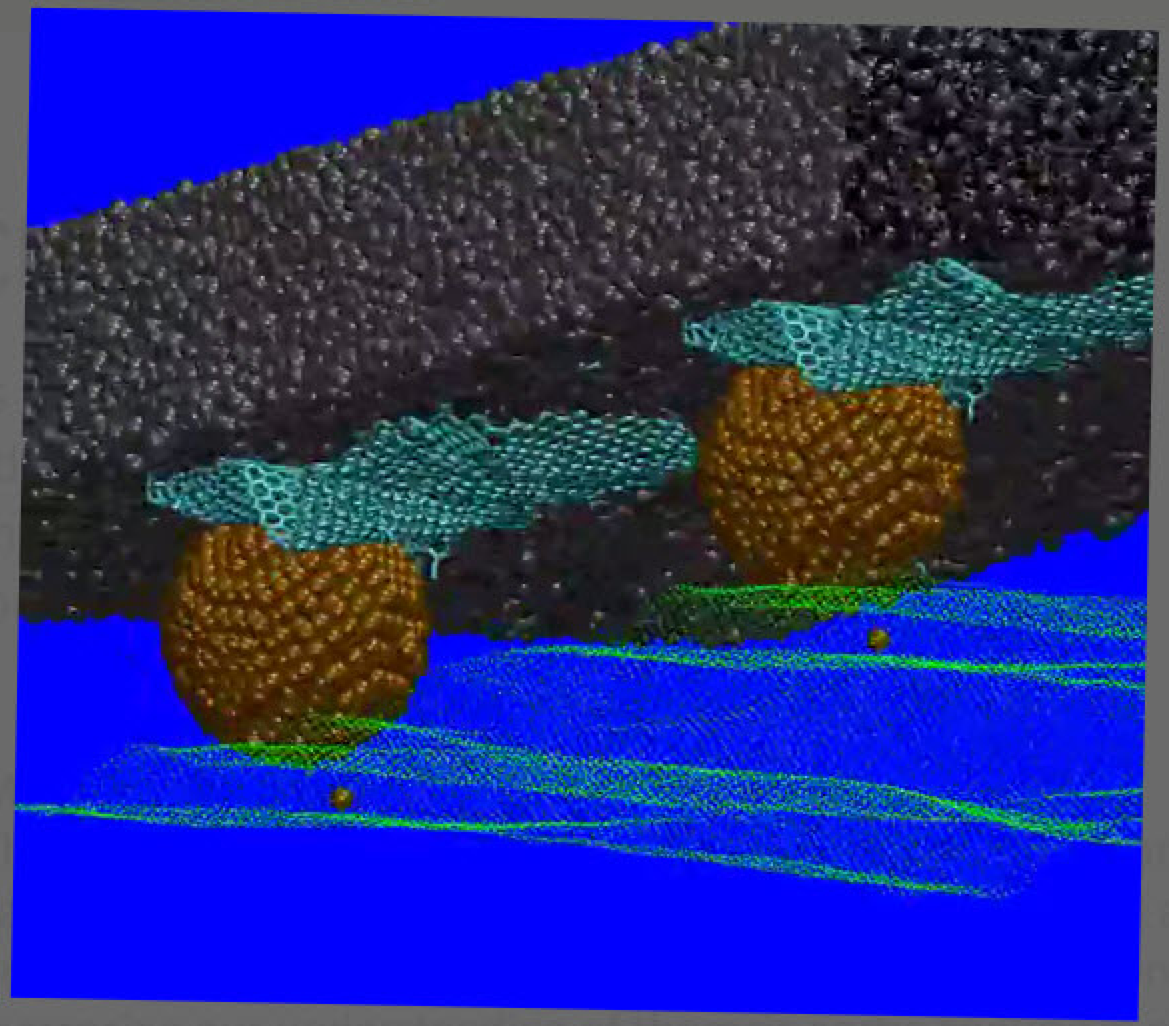

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FUNDING AGENCY: Office of Science

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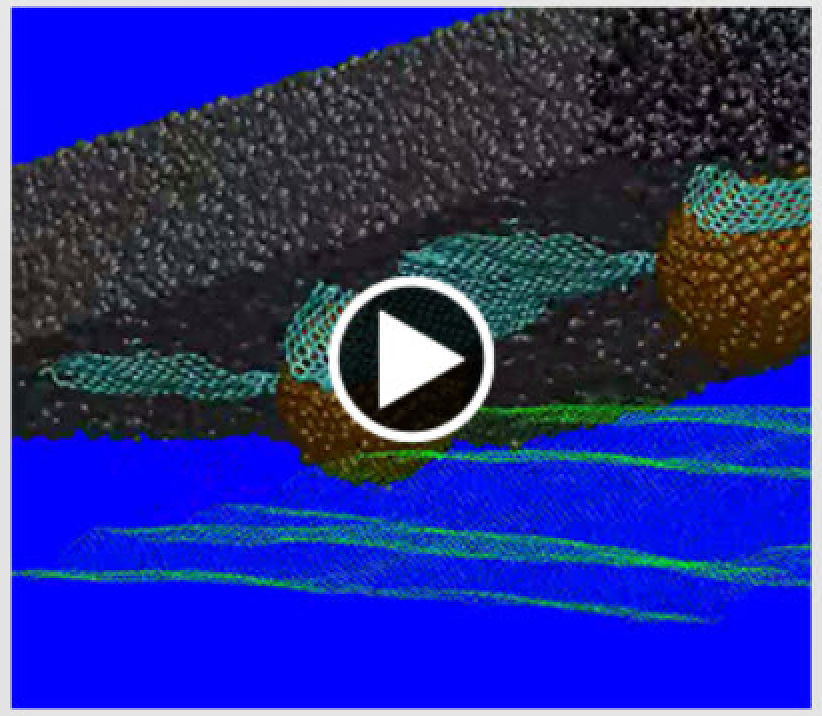
CONTACT: Michael E. Papka, Argonne National Laboratory, papka@anl.gov



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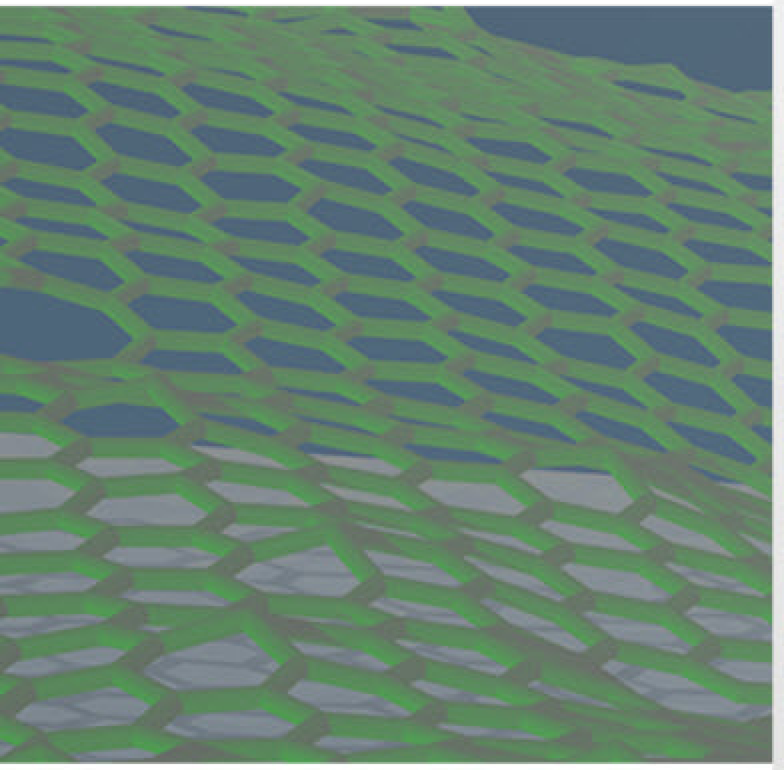

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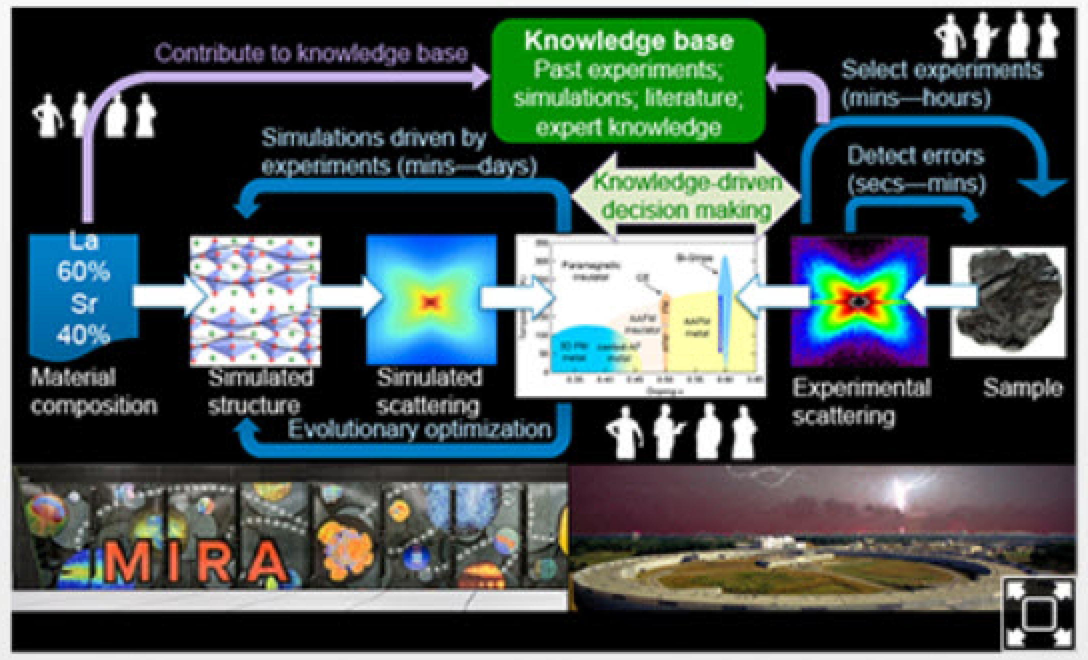
Big Data at Argonne

The capture, management, and analysis of large quantities of data is fundamental to many DOE projects. Argonne researchers in applied mathematics, computer science, and computational science engage in the design, implementation, and application of big data technologies that enable and accelerate discovery in these projects.



Petrel: Data Service for Collaborative Science

This Argonne-developed system supports the staging and rapid dissemination of large datasets. Advanced Photon Source beamlines use Petrel to stage experimental data prior to reconstruction on Argonne Leadership Computing Facility computers and for high-speed access by remote collaborators. Climate researchers use Petrel to distribute climate simulation datasets.

Discovery engines

Argonne research is enabling the creation of new discovery engines that integrate large quantities of data, sophisticated analysis procedures, and powerful numerical simulations to enable more effective experiments and ultimately faster discovery. Argonne teams are developing discovery engines in genomics, material science, cosmology, and other fields.

A unique scientific instrument

The Advanced Photon Source is unique among the world's high-energy X-ray sources in being only a kilometer away from one of the world's most powerful supercomputers. Argonne researchers are leveraging this proximity to pioneer new approaches to high-speed, computer-in-the-loop analysis and steering of experiments.

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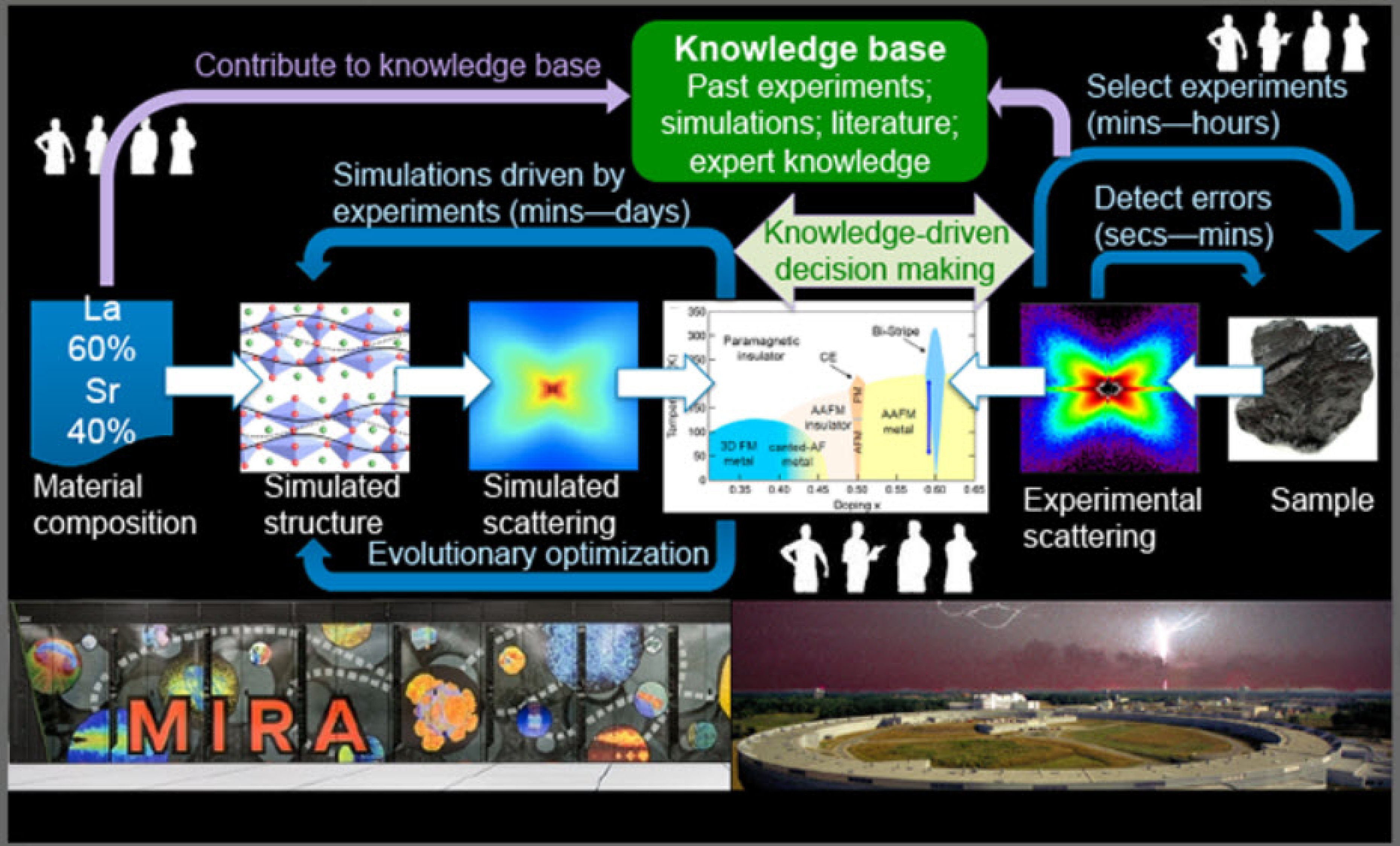

A discovery engine for materials science, showing the integration of experimental and simulation methods to understand the structure of disordered materials.

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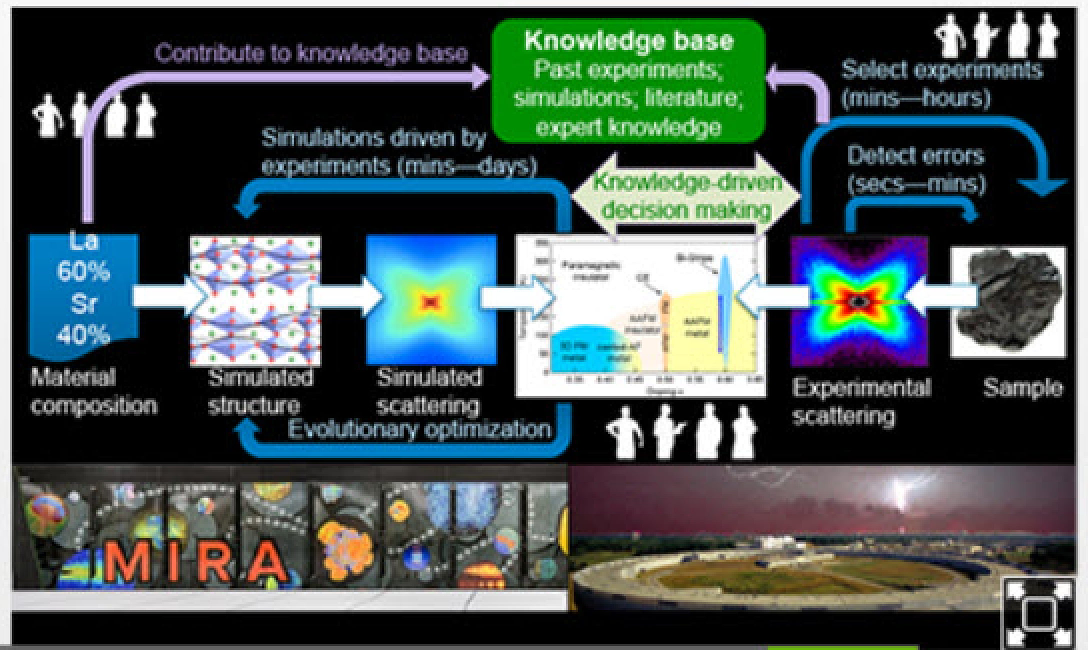

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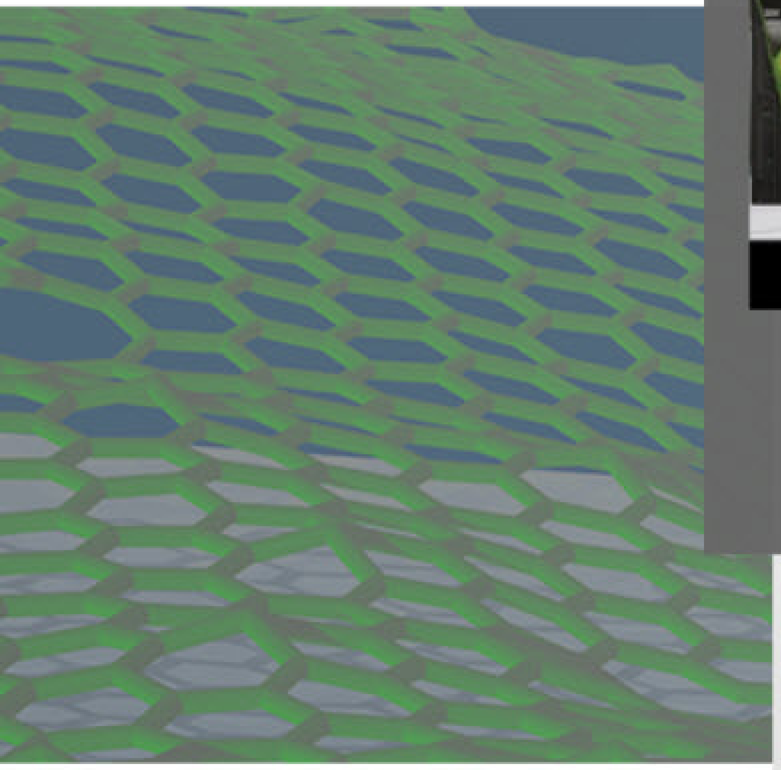

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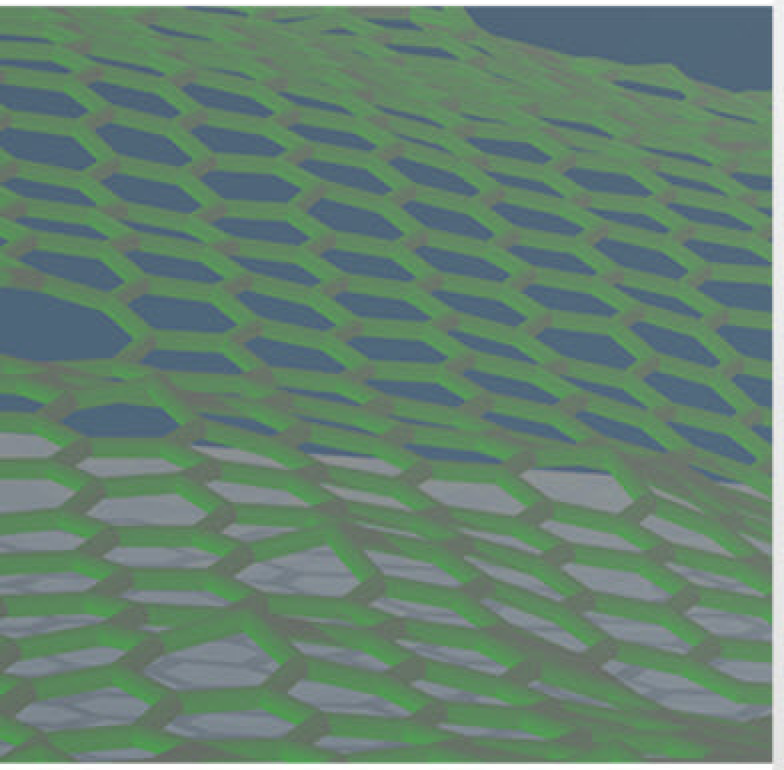
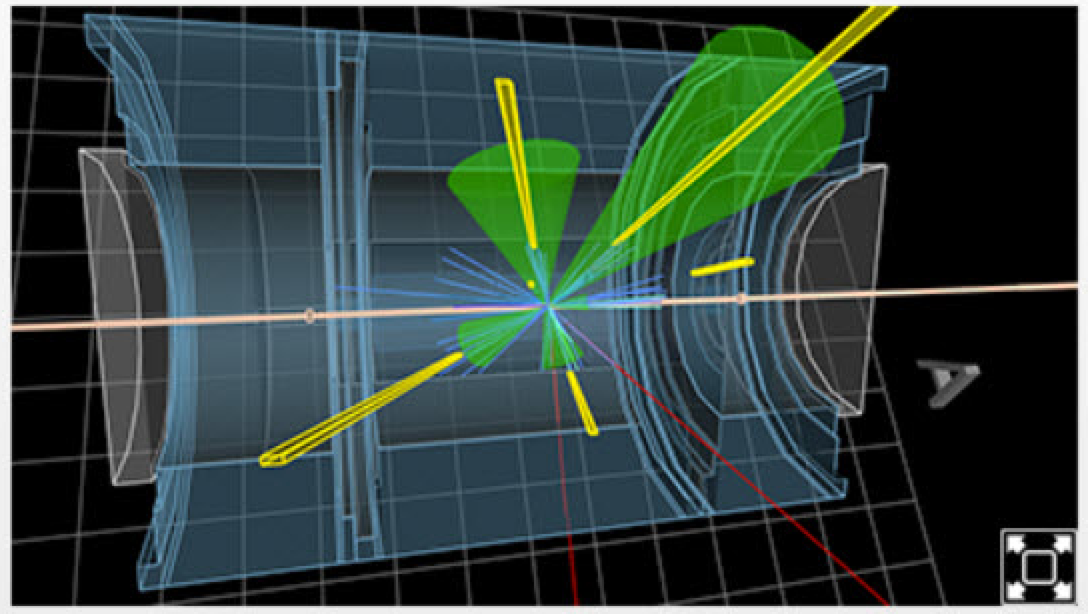


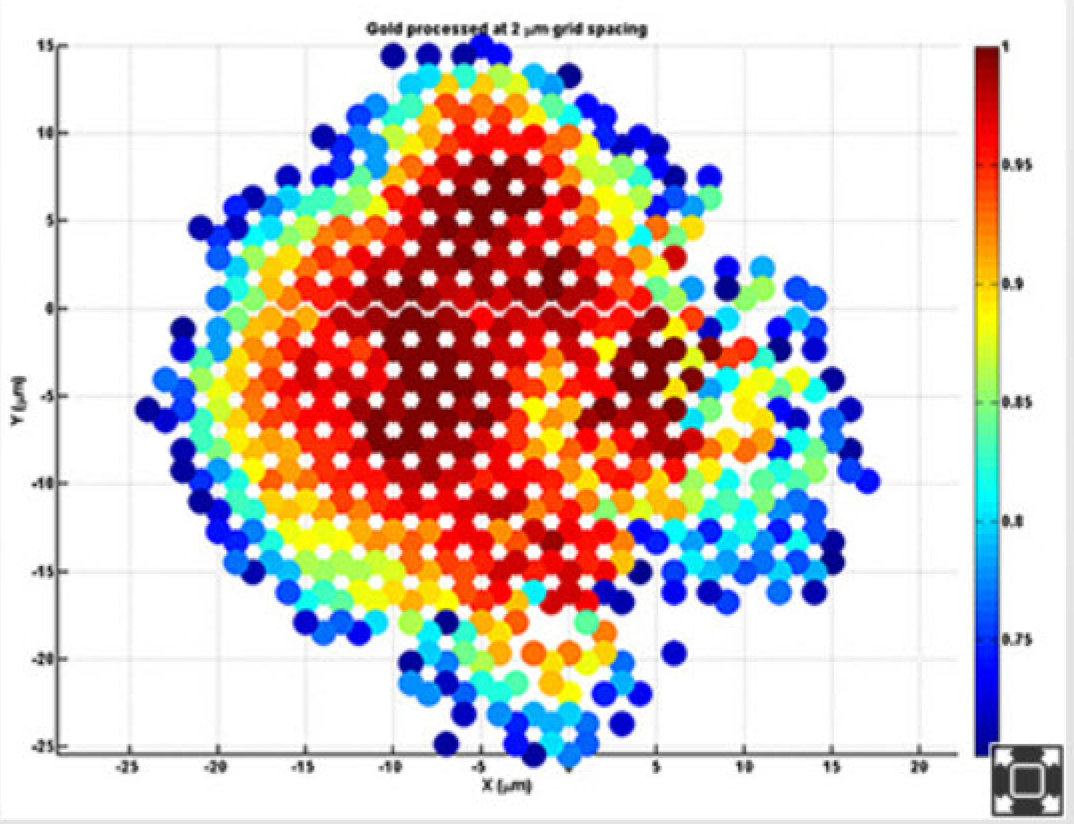
Leveraging ALCF Resources

Argonne researchers are exploring the use of supercomputers as a tool to enable future discoveries at CERN and the Argonne Photon Source. By accelerating the pace at which experimental data can be simulated, these efforts are demonstrating how high-performance computing resources can be used to inform and facilitate data-intensive experiments.



Driving future discoveries at the Large Hadron Collider

For the first time a leadership-class supercomputer is being used to perform massively parallel simulations of LHC collision events. The effort has been a great success thus far, showing that such supercomputers can help drive future discoveries at the LHC by accelerating the pace at which simulated data can be produced. The research also demonstrates how leadership computing resources can be used to inform and facilitate other data-intensive high-energy physics experiments.



Advanced Photon Source Leveraging ALCF Resources

Argonne's Advanced Photon Source (APS) generates the "brightest" high-energy synchrotron x-rays in the Western Hemisphere, enabling scientists to peer inside atomic-level structures and design next-generation materials. This research aims to accelerate discoveries at the APS by leveraging ALCF resources to address gaps in computation, analysis, simulation, and data management for beamline experiments. The team is employing the cyberinfrastructure that is being developed within the project, both for managing data and developing interactive analysis tools and algorithms capable of handling big data.

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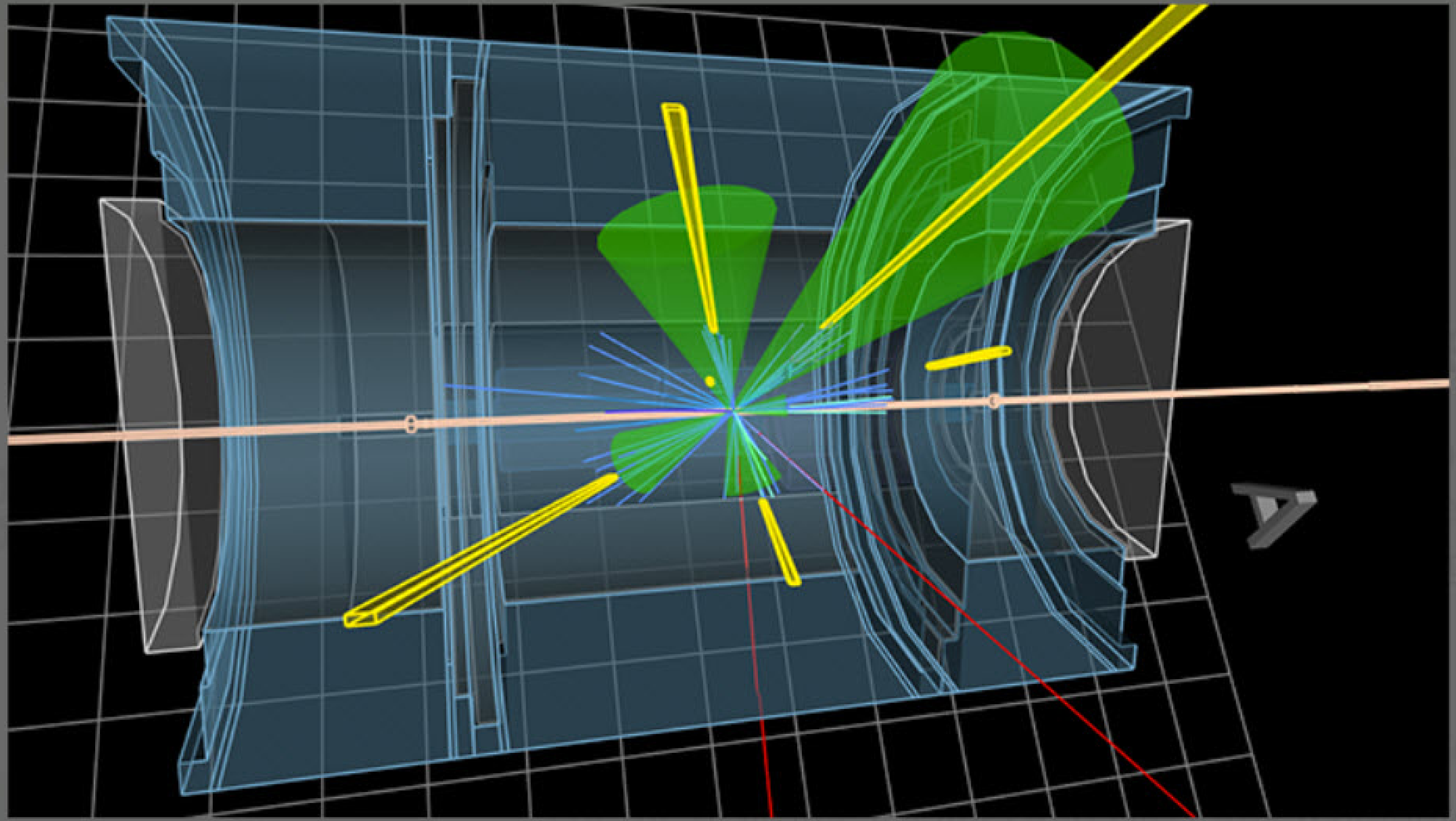
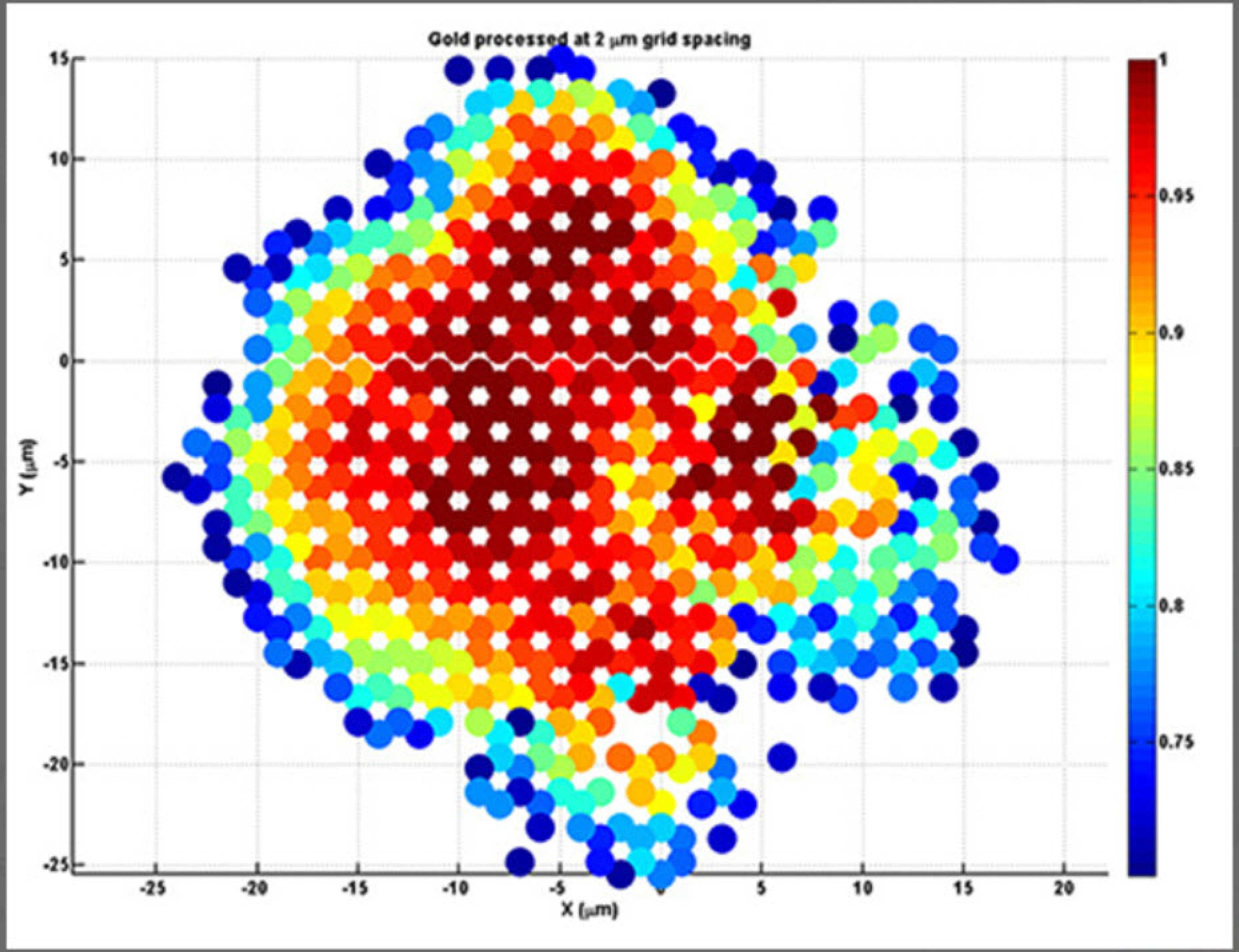


A visualization of a simulated collision event in the ATLAS detector. This simulation, containing a Z boson and five hadronic jets, is an example of an event that is too complex to be simulated in bulk using ordinary PC-based computing grids. Taylor Childers, Argonne National Laboratory



High-energy x-ray diffraction microscopy image of an ~50 micron diameter gold wire (courtesy of B. Suter,Carnegie Mellon University) showing confidence index for each ~1 micron voxel. The data is from the 1-ID beamline of the APS. Reconstructions conducted using APS and ALCF resources were led by Argonne researchers Hemant Sharma and Justin Wozniak. Jonathan Almer and Hemant Sharma, Argonne National Laboratory.

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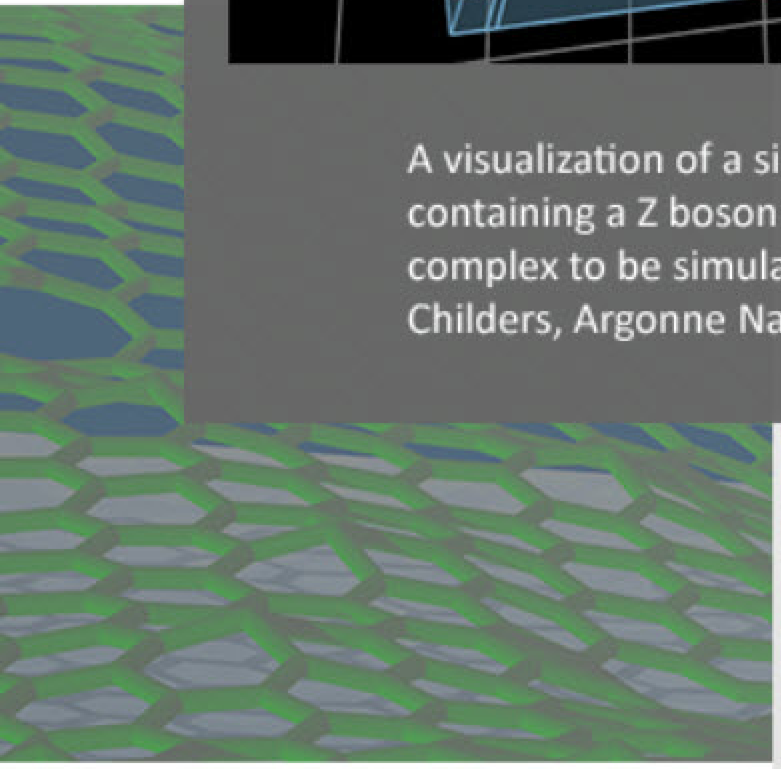

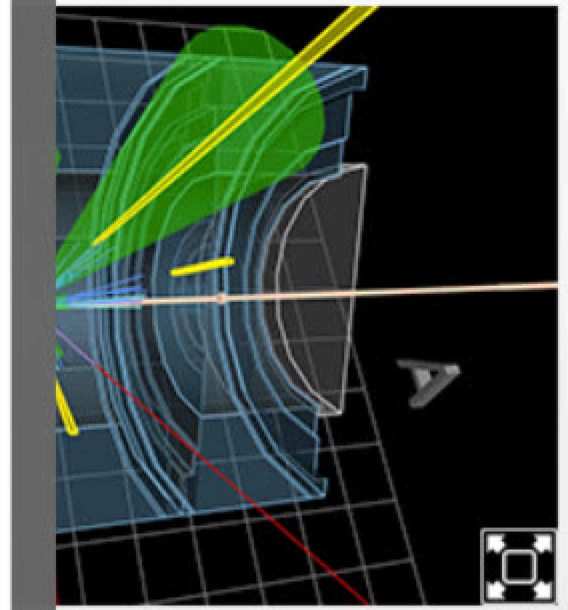

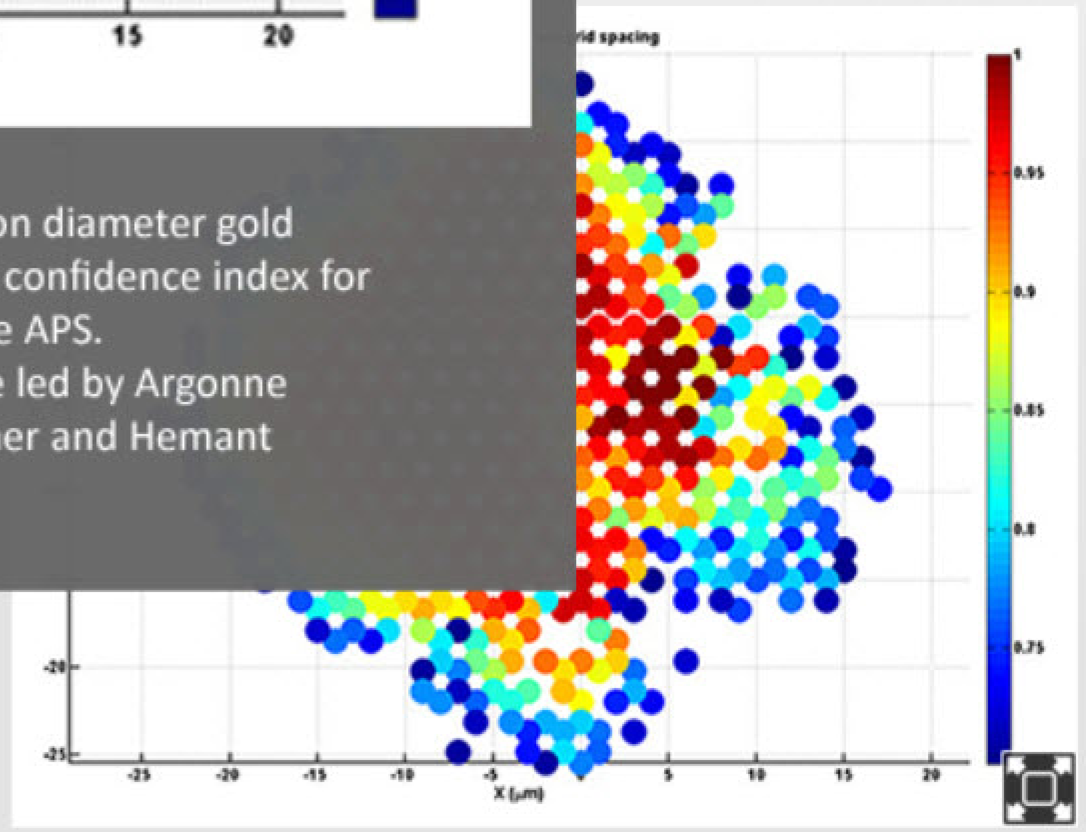

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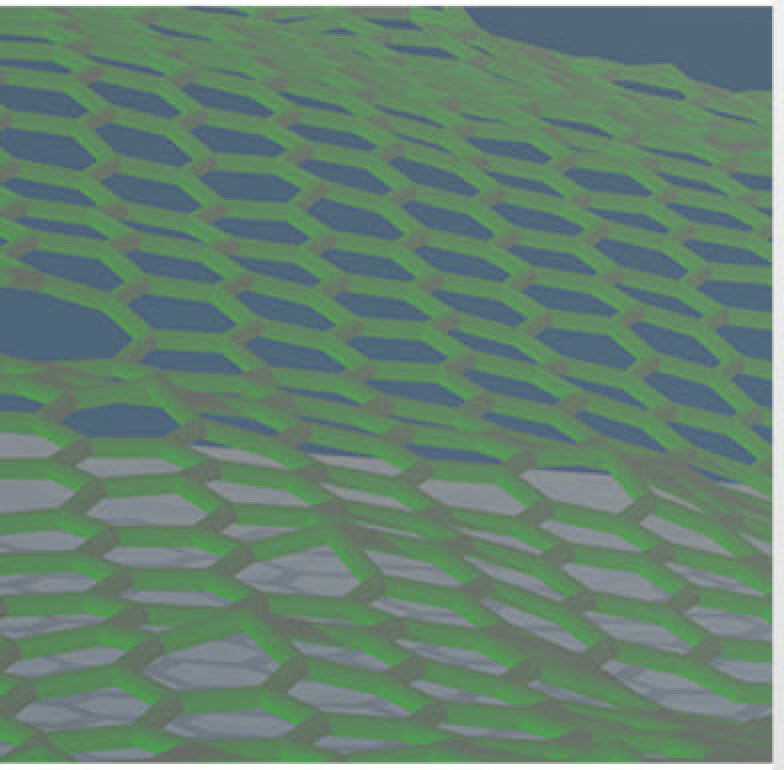

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Applied Mathematics

Innovative Modeling, rigorous theory, transformational algorithms, and scalable software on leading-edge computing platforms

Capabilities
Our work in applied mathematics ranges from modeling of complex phenomena, over rigorous theory and algorithm design, to the development of scalable software tools, to advanced simulations in applications of interest to the U.S. Department of Energy.

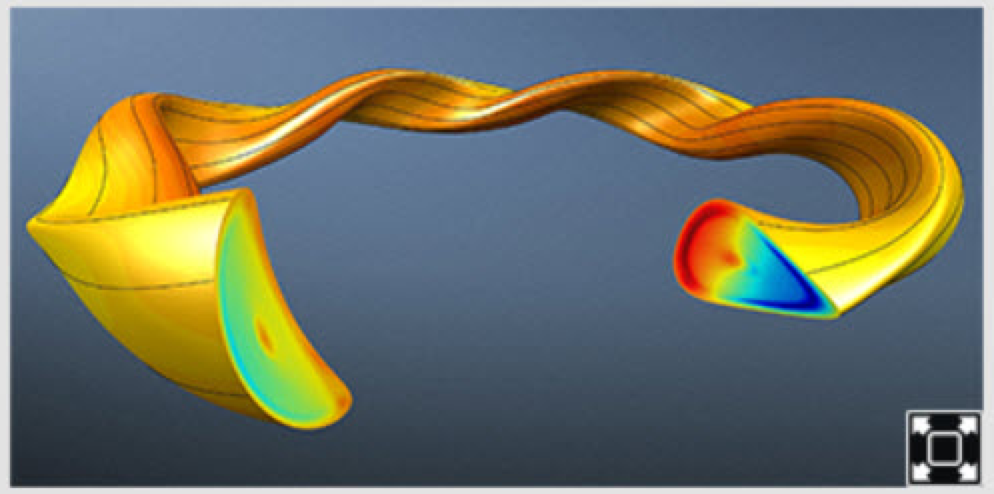
PETSc
PETSc is a suite of data structures and routines for the scalable solution of scientific applications modeled by partial differential equations (PDEs). PETSc is the world's most widely used parallel numerical software library for PDEs, and won an R&D Award in 2009. It tackles diverse applications spanning the breadth of DOE science including biology, fusion, geoscience, nanomaterials, and subsurface flow.

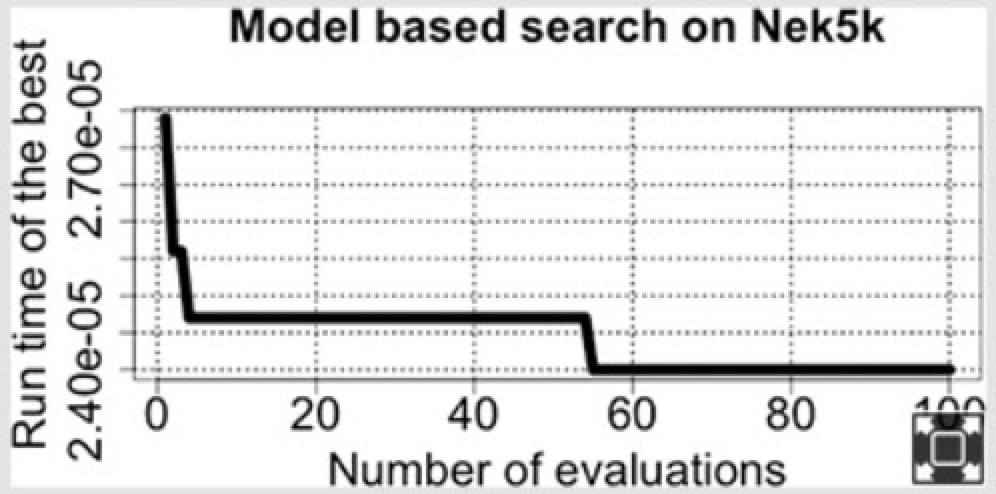
Nek5000
Nek5000 is an open source, highly scalable and portable spectral element code designed to simulate fluid flow, heat transfer and species transport, and magnetohydrodynamics. Nek5000 is a higher-order spectral code that has scaled beyond 500,000 cores on Mira, the IBM Blue Gene/Q supercomputer operated at Argonne (and up to a million cores on Sequoia). Nek5000 received the HPC Innovation Excellence Award at SC'14, and the Gordon Bell Prize in 1999.

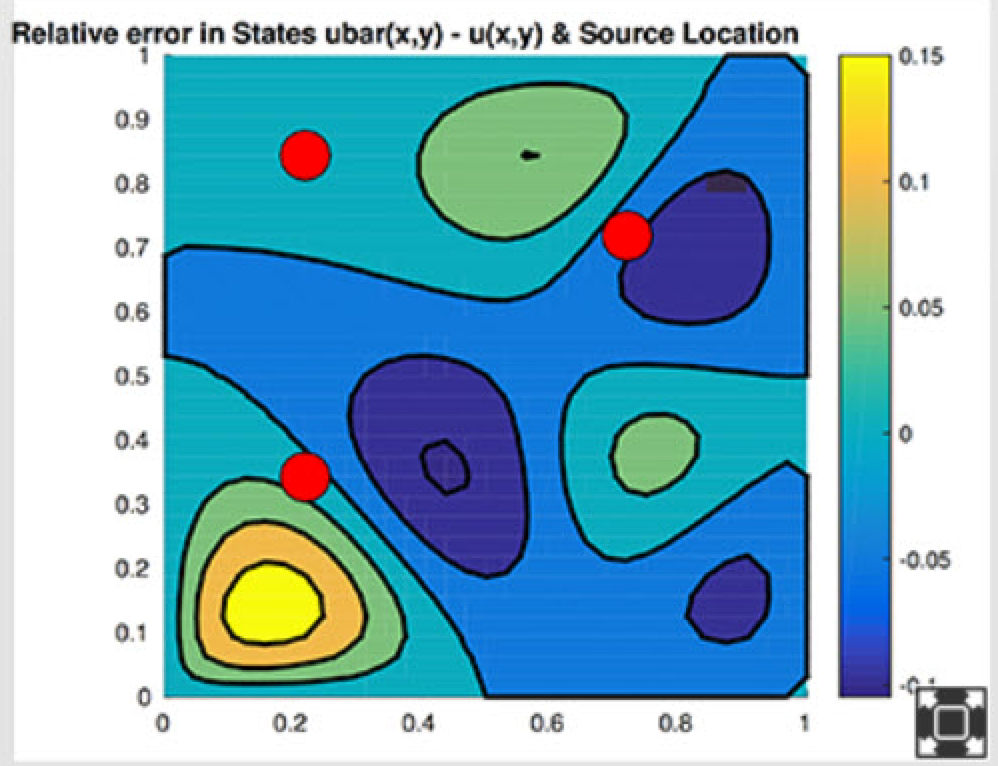
Performance Tuning
We are developing machine-learning tools for autotuning simulation software on different architectures and for tuning design parameters of FPGAs. Our approach develops a surrogate model that is fitted to observed data, and is then optimized with respect to different metrics such as time or energy.

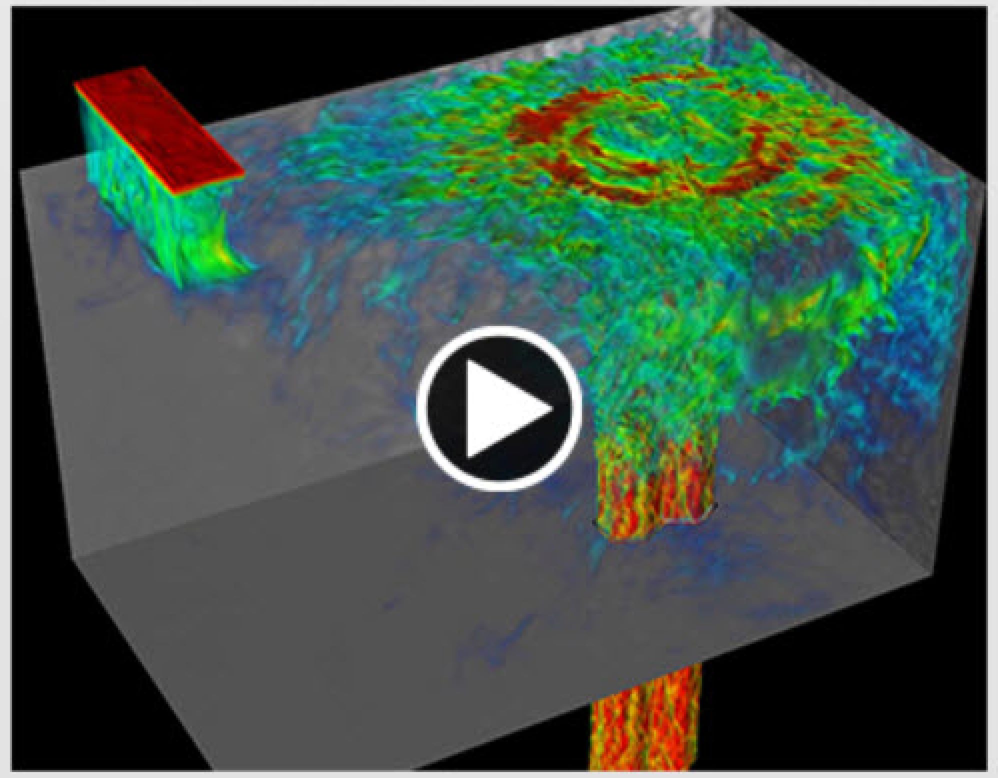
MINOTAUR
Minotaur is an open-source toolkit for solving mixed integer nonlinear optimization problems. It provides different solvers that implement state-of-the-art algorithms for MINLP. The Minotaur library can also be used to customize algorithms to exploit on specific problem structures.

The Future
The applied mathematics program is expanding into new areas of interest to DOE, including new complex inverse problems arising in the analysis of experimental data from DOE light-sources, the modeling of efficient and safe incorporation of renewable energies into the power grid, and optimal performance tuning for high-performance compute resources.

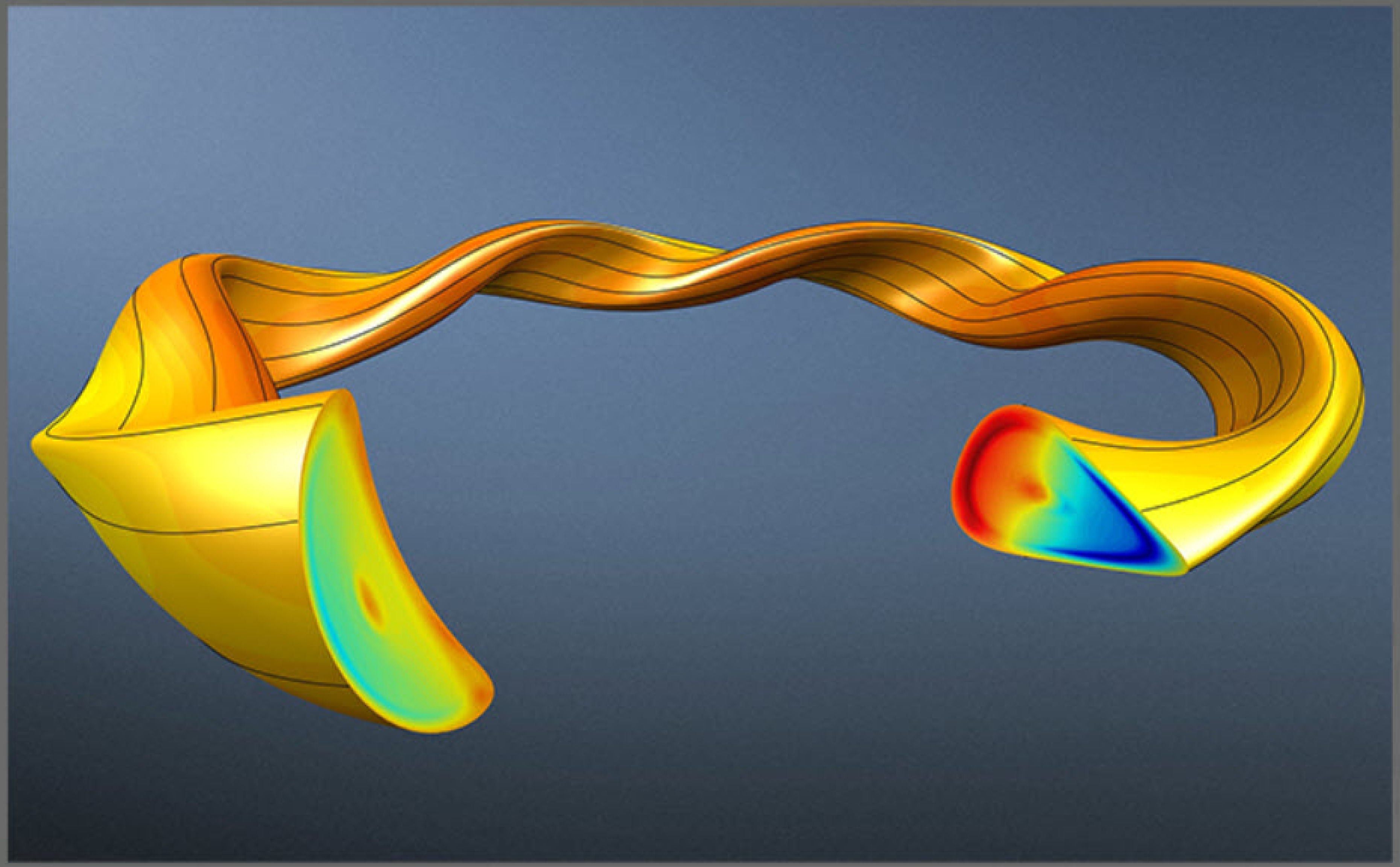




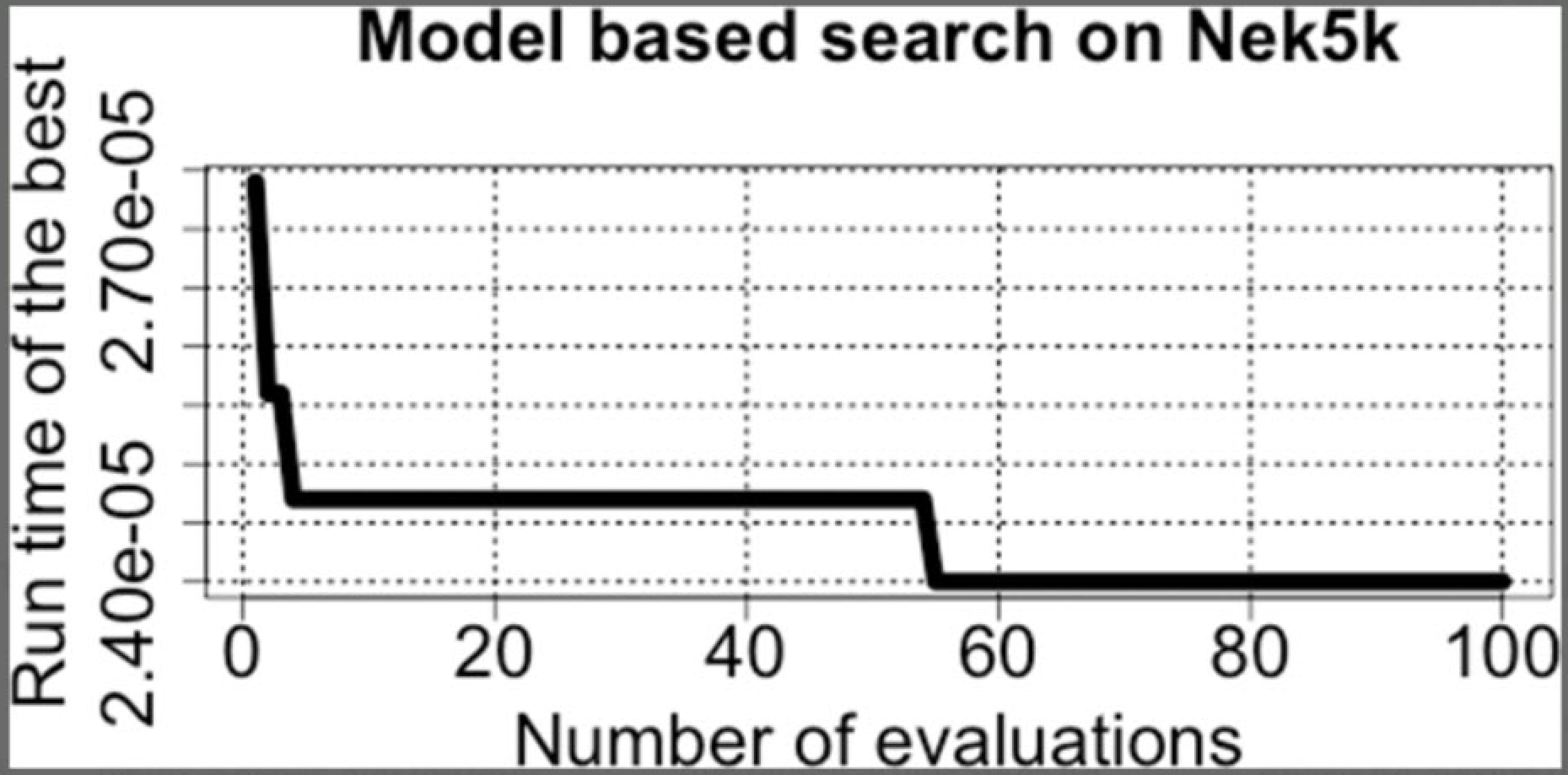




FUNDING & CREDITS



Fokker-Planck kinetic calculation of the parallel current in the W7-X fusion experiment in Greifswald, Germany. Credit: Matt Landreman



Run-time reduction through performance tuning per matrix-matrix multply.

...e computing platforms

spanning the breadth of DOE science including biology, fusion, geoscience, nanomaterials, and subsurface flow.

and magnetohydrodynamics. Nek5000 is a higher-order spectral code that has scaled

FPGAs. Our approach develops a surrogate model that is fitted to observed data, and is then

state-of-the-art algorithms for MINLP. The Minotaur library can also be used to customize algorithms to exploit on specific problem structures.

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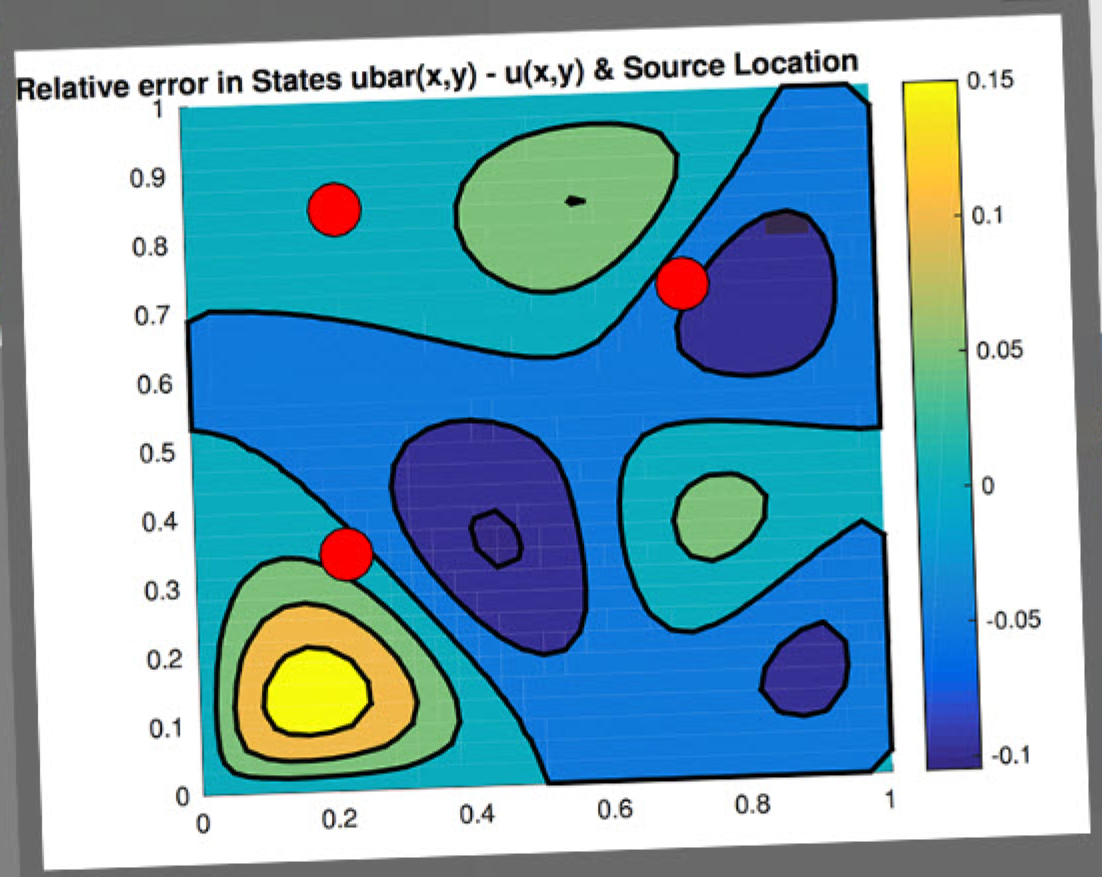
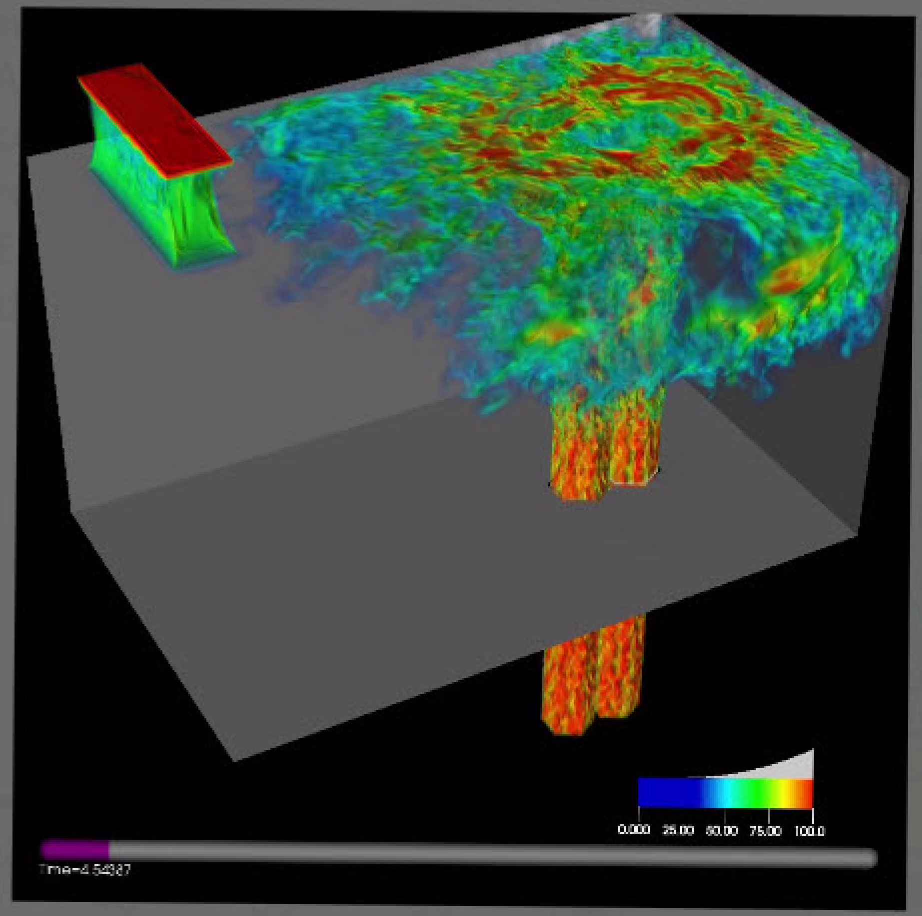


Result of 2D discrete source inversion computed using Minotaur's branch-and-bound framework.



Turbulent flow simulation in mixing chamber of sodium fast reactor to improve outlet design geometry.

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